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

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Tutorials, Joint Symposium and Focus Sessions

- **Tutorial: Modern Photovoltaics - Techniques beyond Silicon (Su)**
- **Tutorial: Physics of NMR - Physics with NMR (Su)**
- **Focus: Structure and Dynamics of Responsive Hydrogels (Mo)**
- **Joint Symposium SYMR: Nuclear Magnetic Resonance - From Applications in Condensed-Matter Physics to New Frontiers (Tu)**
- **Focus: Active Fluids (We)**
- **Focus: Charge Effects in Soft and Biological Matter (Th/Fr)**

Overview of Invited Talks, Topical Talks and Sessions

(lecture rooms H37, H39, H48, H45 (only Th and Fr); Poster B2 and C)

Invited and Topical Talks of CPP Sessions (including Focus Sessions)

CPP 3.1	Mon	10:15–10:45	H37	**Interactive hydrogels** — •Walter Richtering
CPP 3.8	Mon	12:15–12:45	H37	**Dynamics of thermosensitive microgel particles** — •Matthias Ballauff
CPP 4.1	Mon	14:00–14:30	H37	**Current mechanistic and experimental views on the heat-induced phase transition of aqueous poly(N-isopropylacrylamide) solutions.** — •Francoise Winnik
CPP 4.7	Mon	15:45–16:15	H37	**Swelling, structure and hybrid microgel particles** — •Antonio Fernandez-Barbero
CPP 6.1	Mon	11:30–12:00	H39	**Triplet exciton diffusion in organic semiconductors** — •Anna Köhler
CPP 8.1	Mon	11:00–11:30	H48	**Mesoscopic structure formation of polymers in cylindrical nanopores** — •Martin Steinhart
CPP 17.1	Tue	9:30–10:00	H39	**Surviving Structure in Colloidal Suspensions Confined from 3D to 2D** — Yan Zeng, Stefan Grandner, Sabine Klapp, •Regine von Klitzing
CPP 18.1	Tue	13:45–14:15	H39	**Functional thin films based on polymer- and hybrid-nanostructures for photovoltaic applications** — •Peter Müller-Buschbaum
CPP 22.1	Wed	14:00–14:30	H37	**Atomic Layer Deposition (ALD) as a Versatile Tool for Nanoscience** — •Mato Knez, Seung-Mo Lee, Adriana Szeghalmi, Yong Qin, Eckhard Pippel, Christian Dresbach, Gerd Hause
CPP 22.11	Wed	17:00–17:30	H37	**Recognition dynamics and kinetics for ubiquitin** — •Christian Griesinger
CPP 23.1	Wed	9:30–10:00	H48	**On the dynamics of polymers in nanocomposites and under confinement** — •Dieter Richter
CPP 23.2	Wed	10:00–10:30	H48	**From simple liquids to polymers: Dynamics revealed by field cycling ^{1}H NMR** — Axel Herrmann, Azza Abou Elfadl, Roman Meier, Danuta Kruk, Vladimir N. Novikov, •Ernst A. Rössler
CPP 24.1	Wed	14:00–14:30	H48	**New Approach to the Old Problem: Cooperativity in Dynamics of Glass Forming Systems** — •Alexei Sokolov

CPP 24.6	Wed	15:45–16:15	H48	**Slow domains percolation in polymer melts and blends close to the glass transition: a unifying concept regarding bulk dynamics, dynamics in the vicinity of interfaces, and the physical properties of nanocomposites** — •Didier R. Long
CPP 25.1	Wed	9:30–10:00	H39	**Designing small swimmers** — •Ramin Golestanian
CPP 25.2	Wed	10:00–10:30	H39	**Magnetic actuation of paramagnetic colloids at interfaces** — •Thomas Fischer
CPP 25.5	Wed	11:15–11:45	H39	**Active behavior of the cytoskeleton** — •Jean-Francois Joanny, Jacques Prost
CPP 25.6	Wed	11:45–12:15	H39	**Active cytoskeletal polymer networks: from model systems to cells** — •Christoph F. Schmidt
CPP 40.11	Thu	12:15–12:45	H48	**Novel Nanocomposites in Industrial Applications - Chances and Challenges** — •Péter Krüger
CPP 42.1	Thu	11:00–11:30	H39	**Local dynamics near the 2D-Glass Transition in Binary Colloidal Mixtures** — •Georg Maret, Florian Ebert, Sylvain Mazoyer, Peter Keim
CPP 44.1	Thu	9:30–10:00	H45	**Glassy dynamics and charge transport in ionic liquids** — •Friedrich Kremer, Joshua Sangoro, Ciprian Iacob, Jörg Kärger
CPP 45.1	Thu	11:00–11:30	H45	**Charge effects in RNA folding** — •Lois Pollack
CPP 45.3	Thu	11:45–12:15	H45	**Origin of the electrophoretic force on DNA in solid-state nanopores** — •Serge G. Lemay
CPP 46.1	Thu	14:00–14:30	H37	**Electrostatic effects on depletion forces** — •Roberto Piazza, Stefano Buzzaccaro, Jader Colombo, Alberto Parola
CPP 46.6	Thu	15:45–16:15	H37	**In-silico simulation of reentrant protein condensation with highly valent counterions** — Sophie Weggler, Michael Ziller, Fajun Zhang, Frank Schreiber, Oliver Kohlbacher, •Andreas Hildebrandt
CPP 47.1	Fri	10:15–10:45	H45	**Charge inversion in macromolecular systems** — •Christian Holm
CPP 48.1	Fri	10:15–10:45	H39	**Structural arrangement and picosecond dynamics of phospholipids in colloidal systems** — •Tobias Unruh, Sebastian Busch, Martin Schmiele

Invited talks of the joint symposium SYEL - Energy Landscapes: Statistical Physics of (Spin) Glasses, Biomolecules, Clusters, and Optimization Problems

See SYEL for the full program of the Symposium.

SYEL 1.1	Mon	10:00–10:30	H1	**Energy Landscapes of clusters, glasses, and biomolecules** — •David Wales
SYEL 1.2	Mon	10:30–11:00	H1	**Order parameters and energy landscapes for protein folding and misfolding** — •Steven Plotkin
SYEL 1.3	Mon	11:00–11:30	H1	**Nuclear Spins Reveal the Microscopic Nature of Tunneling Systems in Glasses** — •Christian Enss
SYEL 1.4	Mon	11:30–12:00	H1	**Energy landscapes and phase transitions** — •Lapo Casetti
SYEL 1.5	Mon	12:00–12:30	H1	**Phase transitions in spin glasses** — •Peter Young
SYEL 1.6	Mon	12:30–13:00	H1	**Statistical physics of inverse problems** — •Riccardo Zecchina

Invited talks of the joint symposium SYMR - Nuclear Magnetic Resonance: from Applications in Condensed-Matter Physics to New Frontiers

See SYMR for the full program of the Symposium.

SYMR 4.1	Tue	9:30–10:00	H1	**NMR with a Magnetic Resonance Force Microscope** — •Beat H. Meier, Kai Eberhardt, Joss Rosmarie, Tomka Ivan
SYMR 4.2	Tue	10:00–10:30	H1	**Probing Novel Electronic States in Strongly Correlated Electron Materials Using NMR and NQR** — •Nicholas Curro
SYMR 4.3	Tue	10:30–11:00	H1	**Interplay of Structure and Dynamics in Macromolecular and Supramolecular Systems as Revealed by NMR Spectroscopy** — •Hans Wolfgang Spiess
SYMR 4.4	Tue	11:15–11:45	H1	**Big times for small NMR** — •Bernhard Blümich
SYMR 4.5	Tue	11:45–12:15	H1	**Traveling-Wave MRI** — •Klaas Prüssmann
SYMR 4.6	Tue	12:15–12:45	H1	**Life on the Edge: The Origins and Proliferation of Protein Misfolding Diseases** — •Chistopher M. Dobson

Invited talks of the joint symposium SYAT - Anomalous Transport in Heterogeneous Media – from Porous Materials to Cellular Crowding

See SYAT for the full program of the Symposium.

SYAT 1.1	Wed	14:30–15:00	H1	**Aging, ergodicity breaking and universal fluctuations in continuous time random walks: Theory and (possible) experimental manifestations** — •Igor Sokolov
SYAT 1.2	Wed	15:00–15:30	H1	**Distinguishing anomalous from simple diffusion in crowded solutions and in cells with fluorescence correlation spectroscopy** — •Cecile Fradin, Daniel Banks, Shyemaa Shehata, Felix Wong, Robert Peters
SYAT 1.3	Wed	15:30–16:00	H1	**Exploring Diffusion in Nanostructured Systems with Single Molecule Probes: From Nanoporous Materials to Living Cells** — •Christoph Bräuchle
SYAT 2.1	Wed	16:30–17:00	H1	**The Lorentz model: a paradigm of anomalous transport** — •Felix Höfling
SYAT 2.2	Wed	17:00–17:30	H1	**Viscoelastic subdiffusion: from anomalous to normal** — •Igor Goychuk
SYAT 2.3	Wed	17:30–18:00	H1	**Phase transitions, liquid micro-compartments, and embryonic patterning** — •Clifford Brangwynne, Jöbin Gharakhani, Anthony Hyman, Frank Jülicher

Invited talks of the joint symposium SYNT - Nanotribology

See SYNT for the full program of the Symposium.

SYNT 1.1	Fri	10:15–10:45	H1	**Atomic friction under ultrahigh vacuum conditions** — •Ernst Meyer, Enrico Gnecco, Pascal Steiner, Gregor Fessler, Sascha Koch, Thilo Glatzel, Alexis Baratoff, Mircin Kisiel, Urs Gysin, Akshata Rao, Shigeki Kawai, Sabine Maier
SYNT 1.2	Fri	10:45–11:15	H1	**Layering and Squeeze-out Damping in Confined Liquid Films** — •Frieder Mugele
SYNT 1.3	Fri	11:15–11:45	H1	**Wear on the nanoscale: mechanisms and materials** — •Bernd Gotsmann, Mark A. Lantz, Harish Bhskaran, Abu Sebastian, Ute Drechsler, Michel Despont, Yun Chen, Kumar Sridharan, Papot Jaroenapibal, Robert Carpick
SYNT 1.4	Fri	11:45–12:15	H1	**Friction at the Nanoscale: Insights from Atomistic Simulations** — •Izabela Szlufarska, Yifei Mo, Yun Liu, Maneesh Mishra
SYNT 1.5	Fri	12:15–12:45	H1	**The friction of wrinkles** — •Martin H. Müser, Hamid Mohammadi
SYNT 1.6	Fri	12:45–13:15	H1	**Influence of humidity on nano- and micromechanical contact adhesion** — •Hans-Jürgen Butt

Sessions

CPP 1.1–1.5	Sun	16:00–18:30	H2	**Tutorial: Modern Photovoltaics - Techniques beyond Silicon**
CPP 2.1–2.3	Sun	16:00–18:30	H3	**Tutorial: Physics of NMR - Physics with NMR**
CPP 3.1–3.8	Mon	10:15–12:45	H37	**Focus: Structure and Dynamics of Responsive Hydrogels I**
CPP 4.1–4.7	Mon	14:00–16:15	H37	**Focus: Structure and Dynamics of Responsive Hydrogels II**
CPP 5.1–5.4	Mon	10:15–11:15	H39	**New Instruments and Methods**
CPP 6.1–6.4	Mon	11:30–12:45	H39	**Electronic and Optical Properties of Organic Systems I**
CPP 7.1–7.10	Mon	14:00–16:30	H39	**Electronic and Optical Properties of Organic Systems II**
CPP 8.1–8.6	Mon	11:00–12:45	H48	**Crystallization and Self Assembly I**
CPP 9.1–9.10	Mon	14:00–16:30	H48	**Crystallization and Self Assembly II**
CPP 10.1–10.9	Mon	16:30–18:00	Poster C	**Poster: Structure and Dynamics of Responsive Hydrogels**
CPP 11.1–11.11	Mon	16:30–18:00	Poster C	**Poster: New Instruments and Methods**
CPP 12.1–12.10	Mon	16:30–18:00	Poster C	**Poster: Electronic and Optical Properties of Organic Systems**
CPP 13.1–13.10	Mon	16:30–18:00	Poster C	**Poster: Crystallization and Self Assembly**
CPP 14.1–14.29	Mon	16:30–18:00	Poster C	**Poster: Interfaces and Thin Films**
CPP 15.1–15.11	Mon	16:30–18:00	Poster C	**Poster: Nuclear Magnetic Resonance - Frontiers and Applications**
CPP 16.1–16.10	Tue	13:45–16:15	H48	**Nuclear Magnetic Resonance: Frontiers and Applications**
CPP 17.1–17.11	Tue	9:30–12:45	H39	**Interfaces and Thin Films I**
CPP 18.1–18.9	Tue	13:45–16:15	H39	**Interfaces and Thin Films II**
CPP 19.1–19.12	Tue	9:30–12:45	H37	**Organic Electronics and Photovoltaics I**
CPP 20.1–20.10	Tue	13:45–16:15	H37	**Organic Electronics and Photovoltaics II**
CPP 21.1–21.12	Wed	9:30–12:45	H37	**Organic Electronics and Photovoltaics III**
CPP 22.1–22.11	Wed	14:00–17:30	H37	**Biopolymers and Biomaterials (jointly with BP)**
CPP 23.1–23.10	Wed	9:30–12:45	H48	**Polymer Dynamics**
CPP 24.1–24.11	Wed	14:00–17:30	H48	**Glasses and Glass Transition I (jointly with DY and DF)**
CPP 25.1–25.7	Wed	9:30–12:30	H39	**Focus: Active Fluids**
CPP 26.1–26.13	Wed	14:00–17:30	H39	**Micro and Nanofluidics I**
CPP 27.1–27.24	Wed	17:30–19:00	Poster C	**Poster: Organic Electronics and Photovoltaics**
CPP 28.1–28.12	Wed	17:30–19:00	Poster C	**Poster: Biopolymers and Biomaterials**
CPP 29.1–29.3	Wed	17:30–19:00	Poster C	**Poster: Active Fluids**
CPP 30.1–30.16	Wed	17:30–19:00	Poster C	**Poster: Micro and Nanofluidics**
CPP 31.1–31.17	Wed	17:30–19:00	Poster C	**Poster: Polymer Dynamics**
CPP 32.1–32.5	Wed	17:30–19:00	Poster C	**Poster: Liquids and Ionic Liquids**
CPP 33.1–33.7	Wed	17:30–19:00	Poster C	**Poster: Charge Effects in Soft and Biological Matter**
CPP 34.1–34.5	Wed	17:30–19:00	Poster C	**Poster: Elastomers and Gels**
CPP 35.1–35.3	Wed	17:30–19:00	Poster B2	**Poster: Glasses and Glass Transition**
CPP 36.1–36.23	Wed	17:30–19:00	Poster B2	**Poster: Nanoparticles and Composite Materials**
CPP 37.1–37.16	Wed	17:30–19:00	Poster B2	**Poster: Colloids and Complex Liquids**
CPP 38.1–38.5	Thu	9:30–10:45	H39	**Micro and Nanofluidics II**
CPP 39.1–39.11	Thu	9:45–12:30	H38	**Glasses and Glass Transition II (jointly with DY and DF)**
CPP 40.1–40.11	Thu	9:30–12:45	H48	**Nanoparticles and Composite Materials I**
CPP 41.1–41.12	Thu	14:00–17:15	H48	**Nanoparticles and Composite Materials II**
CPP 42.1–42.6	Thu	11:00–12:45	H39	**Colloids and Complex Liquids I**
CPP 43.1–43.14	Thu	14:00–17:45	H39	**Colloids and Complex Liquids II**
CPP 44.1–44.4	Thu	9:30–10:45	H45	**Liquids and Ionic Liquids**
CPP 45.1–45.5	Thu	11:00–12:45	H45	**Focus: Charge Effects in Soft and Biological Matter I (jointly with BP)**
CPP 46.1–46.12	Thu	14:00–17:45	H37	**Focus: Charge Effects in Soft and Biological Matter II (jointly with BP)**
CPP 47.1–47.6	Fri	10:15–12:00	H45	**Focus: Charge Effects in Soft and Biological Matter III (jointly with BP)**
CPP 48.1–48.4	Fri	10:15–11:30	H39	**Colloids and Complex Liquids III**
CPP 49.1–49.8	Fri	10:15–12:15	H48	**Elastomers and Gels**

Annual General Meeting of the Chemical and Polymer Physics Division

Mittwoch 19:15–20:00 H48

- Bericht
- Wahl des stellvertretenden Fachverbandsvorsitzenden
- Frühjahrstagung 2011
- Verschiedenes

CPP 1: Tutorial: Modern Photovoltaics - Techniques beyond Silicon

Chair: Wichard J. D. Beenken, Institut für Physik, Technische Universität Ilmenau

Time: Sunday 16:00–18:30 Location: H2

Tutorial CPP 1.1 Sun 16:00 H2
CdTe thin-film solar cells — •Heinrich Metzner — Institut für Festkörperphysik, FSU Jena, Max-Wien-Platz 1, 07743 Jena

The global industrial production of CdTe solar modules exceeds one Gigawatt per year and so CdTe is probably the most successful thin-film technology of recent years.

In the tutorial, the specific features of the technology are elucidated which make it so competitive. Moreover, the open questions in the materials science of the CdTe-CdS-hetero-structure are discussed and key-issues are identified which are believed to potentially bring the CdTe solar cells to efficiencies well above 20 %.

Tutorial CPP 1.2 Sun 16:30 H2
CIGS thin-film solar cells — •Stefan Paetel — Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden Württemberg (ZSW), Industriestraße 6, 70565 Stuttgart, Germany

This talk covers the current status and understanding of high-efficiency Cu(In,Ga)Se_2 solar cells. Starting with the principal setup of these cells the various parts of the multilayer system will be introduced: substrate, back-contact, absorber, buffer and front contact. This includes the structural, optical and electronic properties of the materials. Furthermore relevant deposition methods are presented along with module manufacturing issues.

Tutorial CPP 1.3 Sun 17:00 H2
Dye-sensitized solar cells — •Sven Rühle — Institute for Nanotechnology and Advanced Materials, Dept. of Chemsitry, Bar Ilan University, Ramat Gan 52900, Israel

Dye-sensitized solar cells (DSSCs) are a low cost alternative to crystalline silicon p-n junction photovoltaic cells. DSSCs consist of a mesoporous nanocrystalline wide bandgap semiconductor (usually TiO_2) that is sintered onto a transparent conducting substrate (TCO). The nanocrystals are covered with a dye-monolayer and the pores are filled with a redox electrolyte which is in contact with a Pt counter electrode. Upon illumination light is absorbed by the dye molecules and electrons are injected from the excited dye state into the TiO_2 conduction band while the dye is regenerated by the electrolyte. Electrons diffuse through the mesoporous film to the TCO front contact while positive charges are transported by the redox species to the counter electrode. In DSSCs efficient charge separation occurs at the TiO_2/dye/electrolyte interface and build-in electrostatic fields play a minor role for cell operation in contrast to p-n junction solar cells. The basic principles of DSSC operation will be reviewed and theoretical efficiency limitations will be discussed.

Tutorial CPP 1.4 Sun 17:30 H2
Organic solar cells based on small molecules — •Moritz Riede — IAPP, Technische Universität Dresden, Germany

In recent years organic solar cells based on polymers or small molecules have received increasing attention from both science and industry, making it a very dynamic field of research. On the one hand, there are a number of open questions on the fundamental physics, e.g. the process of free charge carrier generation. On the other hand, there is the perspective of low cost solar power due to easy solar cell preparation, low-cost materials and processing technologies, and the possibility of producing large-area flexible devices on plastic substrates. Currently there are two main preparation technologies: solution processing and vacuum thermal deposition. This tutorial will focus on the main principles and concepts of the latter one. Despite its limitations to small molecules due to the thermal evaporation process, vacuum deposition has several distinct advantages: small molecules can be purified to a high degree, molecular doping of the organic layers is possible via co-evaporation, the layer thickness can be controlled well and stacked structures, e.g. for tandem solar cells, are easily accessible. Currently, metal-phthalocyanines and C_{60} are used as standard absorbers, but also new and promising materials have been introduced in recent years. Continuous material and device optimisation has lead to certified efficiencies of more than 6% on an device area exceeding 1cm^2. Finally, an outlook on possible production routes is given.

Tutorial CPP 1.5 Sun 18:00 H2
Polymer Solar Cells — •Harald Hoppe — Institut für Physik, Technische Universität Ilmenau, Germany

Milestones in the development of conjugated polymer-based solar cells are reviewed. The presentation will cover an introduction to elementary photo-physical processes and fundamental working principles of polymer solar cells. Furthermore, processes limiting the individual photovoltaic parameters are discussed. Interesting examples of structure-property-relationships on the super-, inter- and intramolecular scale are given and demonstrate the necessity for multi-scale approaches in the optimization of polymer solar cells. Finally, several so far utilized donor-acceptor material systems are briefly reviewed.

CPP 2: Tutorial: Physics of NMR - Physics with NMR

Time: Sunday 16:00–18:30 Location: H3

Tutorial CPP 2.1 Sun 16:00 H3
Spins as Qubits — •Dieter Suter — Fakultät Physik, TU Dortmund

Processing of digital information has progressed at an enormous speed over the last decades and thus become an indispensable resource. Still, for some computational problems, no efficient algorithms are known for today's computers. For some of these problems, an exponential speedup is possible if the computers operate according to Schrödinger's equation, processing the information by unitary transformations. Nuclear spins were the first physical systems used to implement quantum algorithms; in the meantime, several other systems have become available for quantum information processing, all drawing directly from the techniques that NMR has developed for accurately controlling the dynamics of quantum mechanical systems. We will discuss some demonstration experiments that use magnetic resonance techniques to process quantum information stored in nuclear and electronic spins. Since today's quantum computers are based on a small number of qubits, their computational power is quite limited. To make them more powerful, it will be necessary to increase the number of qubits. Many concepts have been proposed that may eventually unlock this potential, some of them based on electronic and nuclear spins.

Literature: J. Stolze and D. Suter, *Quantum Computing: A Short Course from Theory to Experiment*, Wiley-VCH, Berlin, 2nd edition (2008).

short session break

Tutorial CPP 2.2 Sun 17:00 H3
Kernspin-Gitter-Relaxation: Grundlagen, Beispiele, Instrumentierung — •Franz Fujara — Institut für Festkörperphysik, TU Darmstadt, Hochschulstraße 6, 64289 Darmstadt

Im ersten Teil des Vortrags werde ich einige grundlegende Begriffe (Ratengleichungen, Wechselwirkungs-Hamiltonian, Übergangswahrscheinlichkeiten) der elementaren semiklassischen Relaxationstheorie einführen, womit dann Phänomene wie die Relaxationsrate, die Spindiffusion, die Spintemperatur und Fragen der (Nicht)ergodizität diskutiert werden können. Sodann möchte ich instruktive Resultate der traditionellen (Festfrequenz-)Relaxometrie vorstellen, die das Potenzial und die Limitierungen des Verfahrens verdeutlichen. Der letzte Teil des Vortrages behandelt moderne Field-Cycling (FC) Relaxometrieverfahren, sowohl elektronische als auch mechanische. Anhand aktueller experimenteller Beispiele soll ausgeführt werden, dass die FC-Relaxometrie als breitbandiges dynamisches Suszeptibilitätsverfahren betrachtet werden kann, welches mit erheblichem Gewinn gemeinsam mit der Messung anderer dynamischer Suszeptibilitäten, z. B. der di-elektrischen Relaxation oder der dynamischen Lichtstreuung, eingesetzt werden kann.

Tutorial CPP 2.3 Sun 17:45 H3

NMR at High Pressures and High Fields — •Hans Robert Kalbitzer — Institute of Biophysics and Physical Biochemistry, University of Regensburg, D-93040 Regensburg, Germany

The two main methods for biomolecular structure determination are X-ray crystallography and NMR spectroscopy. The major advantage of the former is that virtually no size limit exists for the investigated macromolecules. Yet, only well crystallizeable systems can be analyzed preventing the investigation of for example transient complexes. NMR has the benefit that analysis can be performed in solution under nearly physiological conditions and dynamics can be studied in detail. High pressure NMR has developed in the last decade to a valuable tool for studying biophysical properties of proteins. Static pressure up to 400 MPa is applied to the sample located inside the high-field NMR spectrometer. The pressure is transferred to the sample cell via a pressurizing fluid and can be changed during the experiments. Besides an anisotropic compression of the protein, the most important feature of high pressure NMR spectroscopy is that conformational equilibria can be shifted reversibly, allowing the detection and structural characterization of excited states that are only weakly populated at ambient pressure. Time-dependent non-equilibrium states can be detected by pressure-jump NMR spectroscopy where the pressure is changed repeatedly by approximately 100 MPa in a time scale of 30 ms inside the NMR spectrometer. The pressure response is correlated to NMR parameters by introducing the pressure jumps in a complex pulse sequence (pressure correlation spectroscopy).

CPP 3: Focus: Structure and Dynamics of Responsive Hydrogels I

Time: Monday 10:15–12:45 Location: H37

Invited Talk CPP 3.1 Mon 10:15 H37

Interactive hydrogels — •Walter Richtering — Physical Chemistry, RWTH Aachen University, Aachen, Germany

With macroscopic and microscopic hydrogels it is possible to prepare stimuli sensitive materials that are able to adapt to their environments. We will present examples illustrating how hydrogen bonding and charge interaction can be used to tune properties of hydrogels and microgels both in the bulk and at oil - water interfaces.

CPP 3.2 Mon 10:45 H37

Structure of thermoresponsive polymer hydrogels — •Christine M. Papadakis[1], Joseph Adelsberger[1], Amit Kulkarni[1], Abhinav Jain[1], Andreas Meier-Koll[1], Weinan Wang[1], Achille M. Bivigou-Koumba[2], André Laschewsky[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physikdepartment E13, Garching — [2]Universität Potsdam, Institut für Chemie

Thermoresponsive polymer gels display strong changes in volume when heated above the lower critical solution temperature (LCST). They are thus attractive candidates for e.g. controlled ultrafiltration.

We investigate thermoresponsive polymer hydrogels based on poly(N-isopropyl acrylamide) (PNIPAM) with the focus on the influence of polymer architecture on the morphology. PNIPAM homopolymers as well as diblock and triblock copolymers with a longer PNIPAM block and hydrophobic polystyrene (PS) end blocks are investigated [1]. Structural studies were carried out using mainly small-angle neutron and X-ray scattering (SANS). The homopolymers form a transient gel, whereas the diblock copolymers form a jammed solution of core-shell micelles and the triblock copolymers physically cross-linked micellar networks. The latter constitute an attractive alternative to chemically crosslinked networks.

1. K. Troll, C. M. Papadakis, et al., Colloid Polym. Sci. 2008, 286, 1079. A.M. Bivigou Koumba, A. Laschewsky, et al., Macromol. Chem. Phys. 2009, 210, 565. A. Jain, C. M. Papadakis et al., Macromol. Symp., accepted.

CPP 3.3 Mon 11:00 H37

Salty Microgels – Smart Microgels in Presence of the Hofmeister Series — •Michael Zeiser[1,2], Yvonne Hertle[1,2], Peter Busch[3], and Thomas Hellweg[1,2] — [1]University of Bayreuth, 95440 Bayreuth, Germany — [2]Bayreuth Center for Colloids and Interfaces, 95440 Bayreuth, Germany — [3]Jülich Center for Neutron Science, Forschungs-Neutronenquelle Heinz Maier-Leibnitz, 85747 Garching, Germany

The nature of individual ion properties, so called Hofmeister effects, play a significant role within natural mechanisms. Foaming of ocean water, secondary effects on protein structures and crystallization are just few examples among many.

Smart microgels are networks of colloidal size which are able to respond to external stimuli, such as temperature, by a change in their colloidal dimension. At a certain critical value the particles undergo a volume phase transition. Tuning this volume phase transition can be implemented by changing the chemical composition, solvent etc.. In this study we explored the influence of certain ions on two different thermoresponsive microgel systems. We probed structures and dynamics on different lengthscales by the usage of different light scattering techniques and small angle neutron scattering.

CPP 3.4 Mon 11:15 H37

on the finite-extensibility effect of a single polymer chain — •bing miao[1], thomas a. vilgis[1], stefanie poggendorf[2], and gabriele sadowski[2] — [1]Max-Planck-Institute for Polymer Research, Mainz, Germany — [2]Laboratory of Thermodynamics, Department of Biochemical and Chemical Engineering, Technische Universität Dortmund, Dortmund, Germany

We investigate the finite-extensibility effect on the equilibrium size of a single polymer chain by using a Flory-type calculation. A divergence in the elastic free energy of the polymer chain is introduced to take into account the finite-extensibility. This is of particular importance when considering swelling of polymer networks which is constrained by the finite-extensibility of the polymers. From the analysis of our model, finite-extensibility effect is quantified. Compared to the results of Flory's classic theory, finite-extensibility reduces the equilibrium size of the chain and this effect becomes important for short chains and/or when there exists strong repulsive interaction between monomers of the chain. A typical system of this type is the highly-charged and highly-crosslinked gel.

CPP 3.5 Mon 11:30 H37

New pNIPAM microgels for immobilization of proteins — •Kornelia Gawlitza, Marcel Richter, and Regine von Klitzing — TU Berlin, Stranski-Laboratorium, Strasse des 17. Juni 124, 10623 Berlin, Deutschland

Poly-N-isopropylacrylamide (pNIPAM) belongs to the group of the so called "smart" hydrogels and is one of the most studied water swellable microgel systems. Due to the reversibility of the volume phase transition at around 32°C, pNIPAM is qualified for applications like drug delivery and biocatalysts.[1,2]

In our studies, we synthesized new pNIPAM microgels with suitable properties to reach an immobilization of proteins and hence a new biocatalyst. Therefore, we followed two different strategies: First, we tried to synthesize big hydrogels and second, we used the new comonomer Allylglycine (AG) as anchor points for the enzyme. The characterization of the synthesized microgels was done by Dynamic Light Scattering (DLS) and Atomic Force Microscopy (AFM).

Furthermore, we used the received pNIPAM hydrogels for some immobilization experiments with BSA.[3,4] The following analysis of this experiments was done using the Bradford-assay in combination with fluorescence spectroscopy.

[1] K. Kratz, T. Hellweg, W. Eimer, Polymer (2001), 42, 6531 [2] R. Pelton, Adv. Colloid Interface Sci. (2000), 85, 1 [3] L. Bromberg, M. Temchenko, T. A. Hatton, Langmuir (2003), 19, 8675 [4] C. Yan, A. Elaissari, C. Pichot, J. Biomed. Nanotechnol. (2006), 2(3/4), 208-216

CPP 3.6 Mon 11:45 H37

Temperature sensitivity of colloidal gels measured by multi-speckle DLS — •Martin Medebach, Michael Gradzielski, and Regine v. Klitzing — Stranski Laboratory, Technische Univeristät Berlin, Strasse des 17.Juni 124, 10623 Berlin

We investigated the dynamical behaviour of colloidal systems by the multispeckle DLS method. The multispeckle method is useful to measure the correlation function on a time regime of τ=0.1seconds up to several days. It also provides the possibility to measure time resolved dynamics. Using this method it was found in the past that vesicle gels behaves heterogeneous. In our measurements we could also verify that vesicle gels react sensitive on temperature changes. This could also be the reason of the temporal fluctuations that are visible in distinct τ-channels. This temperature sensitivity was checked in more detail by applying temperature pulses of different amplitudes. The T-sensitivity depends on particle concentration and on how strong the noise is correlated at the measured τ-channel. A system that reacts very sensitive on temperature changes are concentrated PNIPAM microgel particles. The phase transition is detected by the multispeckle method and shows a slowing down of the dynamics at the LCST and a minimum of the noise in the τ-channels. On higher scattering vectors it was possible to do the multispeckle correlation on length scales smaller than the particle size. Here, the fluctuations inside of a particle could be detected at different temperatures.

CPP 3.7 Mon 12:00 H37

Smart Biocompatible Hydrogels constructed with oligo(ethylene glycol) (macro)monomers — Jean-Francois Lutz[1] and •André Laschewsky[2] — [1]Fraunhofer Institute for Applied Polymer Research, Potsdam — [2]University of Potsdam

The main target of our research is to develop novel intelligent polymeric materials for bio-applications. Indeed, synthetic polymers play a key-role in various areas of modern medicine and biotechnology (e.g. bioseparation, controlled drug release, non-viral gene delivery, diagnostics, implants). However, paradoxically, only a few established polymer structures (e.g. PEG, PEI, PLGA, PNIPAM) have been so far widely used in Life Science. In this context, developing new generations of "bio-relevant" macromolecules is an extremely important target, both from a fundamental and technological point of view.

A good example of our synthetic work is our recent design of thermoresponsive polymers based on oligo(ethylene glycol) (macro)monomers. The stimuli-responsive behavior of these new polymers can be precisely controlled by simply varying their molecular structure. Moreover, in comparison to standard thermoresponsive polymers (e.g. PNIPAM) these novel structures possess the advantage to exhibit a reversible phase transition. Hence, we are currently evaluating the potential of these novel biocompatible polymers in various bio-applications. In the present talk, the relevance of this new class of thermoresponsive macromolecules for preparing physically or chemically-crosslinked hydrogels will be discussed.

Invited Talk CPP 3.8 Mon 12:15 H37

Dynamics of thermosensitive microgel particles — •Matthias Ballauff — Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin

We present a survey on recent studies on the dynamics of thermosensitive microgels in aqueous solution. The particles consist of a sold polystyrene core onto which a shell of corsslinked poly(N-isopropylacrylamide) (PNIPA) is grafted. As cores we use spherical particles as well as dumbbell-shaped colloids consisting of two spheres attached to each other. Depolarized dynamic light scattering (DDLS) gives quantitative information about the translational and rotational diffusion coefficient (1). The volume fraction of these particles can be adjusted by the temperature of the system in a continuous fashion. This allows us to study the rheology of such suspension up to high volume fractions. The moduli G' and G" in the linear viscoelastic regime as well as the flow curves as the function of the shear rate are found to be in good agreement with the predictions of mode-coupling theory (2).

1. S. Bolisetty, M. Hoffmann, S. Lekkala, Th. Hellweg, M. Ballauff, L. Harnau, Coupling of Rotation Motion with Shape Fluctuations of Core-Shell Microgels Having Tunable Softness, Macromolecules 2009, 42, 1264-1269
2. M. Siebenbürger, M. Fuchs, H. H. Winter, M. Ballauff, Viscoelasticity and shear flow of concentrated, noncrystallizing colloidal suspensions: Comparison with mode-coupling theory, J. Rheol. 2009, 53, 707-726

CPP 4: Focus: Structure and Dynamics of Responsive Hydrogels II

Time: Monday 14:00–16:15 Location: H37

Invited Talk CPP 4.1 Mon 14:00 H37

Current mechanistic and experimental views on the heat-induced phase transition of aqueous poly(N-isopropylacrylamide) solutions. — •Francoise Winnik — Faculty of Pharmacy and Department of Chemistry, University of Montreal, Montreal, QC Canada

Poly(N-isopropylacrylamide) (PNIPAM) is highly soluble in cold water, but it becomes insoluble as its solution temperature exceeds 32 oC, the lower critical solution temperature (LCST) or cloud point (TCP). This phase transition is governed by the cooperative dehydration of PNIPAM chains and concomitant collapse of individual chains from hydrated coils into hydrophobic globules, which associate to form larger mesoglobules. Recent fundamental and experimental investigations aimed at understanding the physics of the coil-to-globule transition in PNIPAM solutions will be presented with emphasis on the effect of polymer architecture and of additives. [1]

[1] F. Tanaka et al. Phys. Rev.Lett. (2008)101,028302; X.P. Qiu, et al. Macromolecules (2007) 40. 7069.

CPP 4.2 Mon 14:30 H37

Molecular simulation study of the volume transition of hydrogels — •Jonathan Walter[1], Viktor Ermatchkov[1], Jadran Vrabec[2], and Hans Hasse[1] — [1]Laboratory of Engineering Thermodynamics, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Thermodynamics and Energy Technology, University of Paderborn, 33098 Paderborn, Germany

Hydrogels are three-dimensional networks of hydrophilic polymers. The swelling behaviour, one of their most interesting properties, is determined by their network properties and the external conditions. The volume transition of hydrogels mainly depends on the nature of the polymer backbone and the solvent. The cross-linker usually only has a minor influence. This allows studying the volume transition of hydrogel by simulations of the computationally much less expensive polymer strand + solvent system. The volume transition of the hydrogel then corresponds to the change of the polymer strand between its collapsed form in a poor solvent and its stretched form in a good solvent. Here, the swelling and collapsing of Poly(N-isopropylacrylamide) is studied by molecular dynamics simulation on the basis of transferable all-atom and united-atom force fields using explicit solvent models from different literature sources. This work focuses on the influence of the temperature and solvent composition on the volume transition of the hydrogel. It is shown that the molecular simulations allow qualitative predictions of the swelling behaviour observed in experiments.

CPP 4.3 Mon 14:45 H37

Thermodynamics of aqueous solutions containing N-isopropyl acrylamide hydrogels — •Viktor Ermatchkov, Luciana Ninni Schäfer, and Gerd Maurer — Laboratory of Engineering Thermodynamics (LTD), Department of Mechanical and Process Engineering, University of Kaiserslautern, D-67653 Kaiserslautern, Germany

Applications of hydrogels are based on their physico-chemical properties, among which the swelling behavior is one of the most important. The development of models for a reliable description of the phase equilibrium in systems containing hydrogels requires quantitative experimental data on the swelling behavior of well-characterized hydrogels.

In previous work, the phase equilibrium and swelling properties of some synthetic hydrogels was determined and quantitatively described by combining expressions for the Gibbs energy of an aqueous solution of polymers and for the Helmholtz energy of an elastic network. The hydrogels consisted of a single nonionic monomer N-isopropyl acrylamide (NIPAAm) as well as of mixtures of NIPAAm and anionic comonomer (sodium methacrylate). In the current work these investigations are extended to other (NIPAAm)-hydrogels, in particular to hydrogels with two ionic comonomers of different charges (2-Acryloylamino-2-methylpropane-1-sulfonic acid and N-[3-(dimethylamino)propyl]-2-methylprop-2-enamide) and to hydrogels containing also a zwitterionic comonomer (3-(dimethyl{3-[(2-

methylacryloyl)amino]propyl}ammonio)propane-1-sulfonate).

New experimental results for the swelling of such hydrogels in aqueous solutions as well as model extensions are presented.

CPP 4.4 Mon 15:00 H37

Free volume and swelling in thin films of poly(N-isopropylacrylamide) end-capped with n-butyltrithiocarbonate — •Stephan Harms[1], Klaus Rätzke[1], Franz Faupel[1], Werner Egger[2], Luca Ravelli[2], André Laschewsky[3], Weinan Wang[4], and Peter Müller-Buschbaum[4] — [1]CAU Kiel, Institut für Materialwissenschaft - Materialverbunde — [2]Universität der Bundeswehr München — [3]Potsdam Universität, Inst. Chemie — [4]TU München, Physik-Department LS E13

Thin hydrogel films of poly(N-isopropylacrylamid) end-capped with n-butyltriocarbonate (nbc-PNIPAM) show a thickness dependent swelling behavior, i.e. the thinner the films, the more they can swell, normalized to the respective thickness [1]. A tentative explanation is centered on differences in free volume. As the o-Ps lifetime is a generally accepted measure for the average free volume, positron annihilation lifetime spectroscopy as function of energy is performed to obtain depth profiles of the free volume of nbc-PNIPAM films with thicknesses from 40 to 200 nm. The results clearly show higher o-Ps lifetimes and hence higher free volume for thinner films. Results are discussed with respect to free volume and mobility influences on sorption and swelling behavior.

[1] Wang W., Troll K., Kaune G., Metwalli E., Ruderer M., Skrabania K., Laschewsky A., Roth S.V., Papadakis C.M., Müller-Buschbaum P.; Macromolecules 2008, 41, 3209

CPP 4.5 Mon 15:15 H37

Crosslinking and Patterning of Sensitive Polymers with Electron Beam Lithography: Sensoric Application — •Claudia Kaiser[1], Ingolf Moench[2], and Karl-Friedrich Arndt[1] — [1]Physical Chemistry of Polymers, Department of Chemistry, TU Dresden, 01062 Dresden, Germany — [2]Leibniz-Institute for Solid State and Materials Research Dresden, Germany

Sensitive hydrogels provide an excellent basis for various industrial applications due to their ability to change conformation in response to even a little change in environmental conditions (e.g. temperature, concentration of a second component or pH). Examples are optoelectronics, fluidics or pharmaceutics. A further possibility offers the integration in sensor systems. Miniaturization of hydrogel patterns is a basic requirement for application in microsystems. Thus, latest researches are engaged in the synthesis and characterization of hydrogel structures in the μm and 100 nm scale. The aim of our work is to give an overview about the possibilities to pattern several stimuli-sensitive polymers with electron beam lithography. We present results concerning synthesis, structuring parameters, attained dimensions, and the retained sensitivity by measuring property changes. To show the variability of the technique we investigate the polymers hydroxypropylcellulose, PNIPAM, P4VP, pluronic F127, and PVA/PAA-blend. For different application, e.g. to monitor the swelling-/deswelling-process by measurement of corresponding signals it could be useful to functionalize the polymer layer by filling. Therefore, the polymer layers become filled with different nanoparticles.

CPP 4.6 Mon 15:30 H37

Structure and response of pNIPAM microgels loaded with gold particles under thermal and optical stimuli — •Adrian Carl and Regine von Klitzing — Stranski-Laboratorium, Institut für Chemie, Technische Universität Berlin, Strasse des 17. Juni 124, 10623 Berlin

Gold particles as well as pNIPAM microgels have been studied separately over the last decade. We studied the changes in thermal and optical responsivity of several composite particles compared to the properties of separate materials. Gold nanospheres and nanorods (AuNPs) were synthesised in the presence of pNIPAM microgels which contain different amounts of charged comonomers.

The influence of the gold particle shape and particle number on the swelling behaviour was studied by DLS measurements at two different wavelengths to investigate possible surface plasmon resonance effects. In order to obtain information about the distribution of the AuNPs inside of the microgel network, AFM, TEM and SAXS measurements were applied. During the phase transition of the microgels from swollen to collapsed state in the temperature range of 30-40°C (depending on the comonomers used), a wide broadening of the SPR-band in the UV-VIS spectra indicated a strong reversible interaction of the AuNPs.

The optical responsivity was further examined by turbidity measurements and a 2-laser DLS apparatus.

[1] Karg, M. Pastoriza-Santos, I. Rodriguez-Gonzalez, B.; von Klitzing, R. Wellert, S. Hellweg, T. Langmuir 2008, 24, 6300-6306

[2] Eustis, S. El-Sayed, M. A. Chem. Soc. Rev. 2006, 35, 209-217

Invited Talk CPP 4.7 Mon 15:45 H37

Swelling, structure and hybrid microgel particles — •Antonio Fernandez-Barbero — Department of Applied Physics, University of Almería, 04120-Almería, Spain

Different aspects about the swelling of individual microgel particles are revised: thermodynamics, microscopic structure, colloidal aggregation, solvent confinement,..., as well as discontinuous transitions. The structure of dense colloidal suspensions containing microgel particles will be discussed. Finally, the properties of different material are combined to design and fabricate hybrid particles with modulated response.

CPP 5: New Instruments and Methods

Time: Monday 10:15–11:15 Location: H39

CPP 5.1 Mon 10:15 H39

Investigation of hybrid nanostructures using AFM/STM based on tuning fork sensors — •Inshad Jum'h, Viatcheslav Dremov, Yuri Koval, and Paul Müller — Department of Physics and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg

We present a combination of non-contact AFM and STM using a sharp etched metal tip and a quartz tuning fork as the force sensor. This method has proven to be stable at ambient conditions and provides high-resolution images of topography, conductivity, force gradient and dissipated power simultaneously. This is suitable for conductive, partially conductive and nonconductive materials. In this work, we study a variety of nanostructures and map the conductivity of various hybrid materials. We present our recent results for the graphitized layer of polymer surfaces modified by low energy ion beam irradiation. We demonstrate the possibility to study composite materials based on few layered graphite (FLG) using this method.

CPP 5.2 Mon 10:30 H39

Nanomechanical characterization of fibrillar structures — •Daniel Kluge and Andreas Fery — Department of Physical Chemistry II, Universität Bayreuth, Universitätsstraße 30, 95440 Bayreuth, Germany

Micro- and nanofibers have become increasingly important in materials sciences as there are many diverse applications for tissue engineering, filtration and in composite materials. The most fundamental requirement for all of these applications is a suitable mechanical stability. In order to investigate the mechanical properties of small-scale fibers, approaches beyond standard characterization methods for macroscopic materials are necessary. Recently, we studied the nanomechanical properties of self-assembled 1,3,5-tris(2,2-dimethylpropionylamino)benzene fibers. For that purpose, we developed a new approach on AFM bending experiments that used force mapping to acquire spatially resolved force measurements over the full length of a free standing fiber segment. This allowed us the validation of the experimental boundary conditions directly from the AFM data and a reliable determination of Young's modulus. In this contribution, we will present our technique and discuss its application for other fibrillar systems.

CPP 5.3 Mon 10:45 H39

Temperature Measurements within a Laser Heating Process on Polymer Films — •Ralf S. Kappes[1] and Jochen S. Gutmann[1,2] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Joh.-Gutenberg University, Mainz, Germany

There are multiple ways of measuring temperatures nowadays. Still the task of detecting high temperatures, i.e. around 1000 Kelvin with a microsecond time and a micrometer size resolution is quite challenging. However, the temperature is an important factor if it comes to the understanding of processes which proceed in those orders of magnitude, like for example laser heating on polymer films. To achieve this goal we set up an optical detection system using high performance optics and a microsecond gated camera in combination with various interference filters to detect the thermal emission spectrum in the Vis range. Analyzing the radiation data via a fit of Planck's law to the obtained curve we are finally able to collect a 2D temperature profile for time intervals as short as one microsecond within a process. In this way we can show, that a polymer film, which is doped with an organic dye for energy conversion, can reach temperatures of at least 900 Kelvin, which is high above its "normal" decomposition temperature, determined e.g. from thermogravimetric methods. And it is furthermore possible for us to achieve a relation between the temperature in process and the effect on the polymer film afterwards.

CPP 5.4 Mon 11:00 H39

Hyperspectral CARS imaging of polyolefine deformation — •Gregor Hehl[1], Gulnara Yu. Nikolaeva[2], Stefan Gomes da Costa[1], and Andreas Volkmer[1] — [1]3rd Institute of Physics, University of Stuttgart — [2]RAS, Moscow, Russia

We report on the hyperspectral coherent anti-Stokes Raman scattering (CARS) imaging of the initial stages of polyolefine deformation. Many polyolefines undergo uniaxial stretching with formation of a so-called necking region where the axes of most of the macromolecules become oriented along the direction of deformation [1]. To investigate the structural changes of macromolecular orientation without perturbing the polymer structure of interest, labelfree hyperspectral CARS imaging [2] of polyethylene and isotactic polypropylene was performed. Spectral CARS hypercubes providing both spectral and spatial information of the polymers for each image voxel have been collected with 5-cm-1 and sub-micron resolution, respectively. Based on the corresponding phase-retrieved Raman hypercube using the Maximum Entropy method [3] and on the characteristic Raman bands of the polymers, hyperspectral data processing results in pseudo-color images of the degrees of molecular orientation and of crystallinity. Unlike conventional X-ray measurements, IR and Raman microspectroscopies, we demonstrate unprecedented fast 3D chemical mapping of local physical structure information of polymers with high spatial resolution and at high spectrum acquisition rate. [1] S. A. Gordeev et al., Polymer Science, Ser. A 38 (1996), 517, [2] A. Volkmer, J. Phys. D: Appl. Phys. 38 (2005), R59, [3] E. Vartiainen et al., Appl. Spectrosc. 50 (1996), 1283.

CPP 6: Electronic and Optical Properties of Organic Systems I

Time: Monday 11:30–12:45 Location: H39

Topical Talk CPP 6.1 Mon 11:30 H39

Triplet exciton diffusion in organic semiconductors — •Anna Köhler — Department of Physics, University of Bayreuth, Bayreuth, 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 use a series of poly(p-phenylene)-type conjugated polymers and oligomers of variable degree of molecular distortion (i.e. polaron formation) and energetic disorder as model systems to study the Dexter-type triplet exciton diffusion in thin films. We show that triplet diffusion can be quantitatively described in the framework of a Holstein small polaron model (Marcus theory) that is extended to include contributions from energetic disorder. The model predicts a tunnelling process at low temperatures followed by a thermally activated hopping process above a transition temperature. In contrast to charge transfer, the activation energy required for triplet exciton transfer can be deduced from the optical spectra. We discuss the implications for device architecture.

CPP 6.2 Mon 12:00 H39

Selective excitation of exciton transitions in PTCDA crystals and films — •Reinhard Scholz[1], Linus Gisslen[1], Venkat R. Gangilenka[2], Lyubov V. Titova[2], Leigh M. Smith[2], L. A. Ajith De Silva[3], and Hans-Peter Wagner[2] — [1]Walter Schottky Institut, Technische Universität München — [2]Department of Physics, University of Cincinnati — [3]Department of Physics and Geology, Northern Kentucky University

Photoluminescence excitation studies on 3,4,9,10-perylene tetracarboxylic dianhydride (PTCDA) single crystals and polycrystalline PTCDA films are compared to the calculated excitonic dispersion deduced from an exciton model including the coupling between Frenkel excitons and charge transfer (CT) along the stacking direction. For excitation energies below the 0-0 Frenkel exciton absorption band at 5 K, these measurements enable the selective excitation of several CT states. The CT2 state involving stacked PTCDA molecules gives an excitation resonance for photoluminescence from the self-trapped CT2 exciton and from the non-relaxed CT2-nr state. Moreover, the fundamental transition of the CT1 involving both basis molecules in the crystal unit cell can be determined from the respective excitation resonance. The excitation energy dependence of the different emission bands allows the assignment of the fundamental transition energies of the CT2 and CT1 excitons to 1.95 eV and 1.98 eV, respectively. When the excitation energy exceeds 2.10 eV, we observe a dominating emission channel related to the indirect minimum of the lowest dispersion branch dominated by Frenkel excitons.

CPP 6.3 Mon 12:15 H39

A new dimension in controlling ultrafast exciton dynamics of mesoscopic chromophore aggregates by fractal geometry — •Dmitri V. Voronine — Institut für Physikalische Chemie, Universität Würzburg, Würzburg, Germany

Ultrafast exciton percolation dynamics in mesoscopic chromophore aggregates was investigated using femtosecond transient absorption spectrometry. Ultrashort laser pulse excitation resulted in exciton-exciton annihilation whose rate depends on the spectral dimension of inhomogeneously broadened aggregates. The value of the spectral dimension and, therefore, the geometry of exciton percolation pathways can be controlled by varying the fractal aggregate geometry which is characterized by the fractal dimension. The fractal geometry dependence was shown for two types of porphyrin homo-aggregates: cationic (Pagg) and anionic (TPPS) porphyrins. The possibility to control the fractal and spectral dimensions of a porphyrin hetero-aggregate was also investigated. These results might be useful for the design of new materials for artificial light harvesting applications and for a better understanding of exciton dynamics in analogous systems such as conjugated polymers, carbon nanotubes, and others.

CPP 6.4 Mon 12:30 H39

Absorption and Emission Spectroscopic Characterisation of 8-Amino-Riboflavin — •Amit Tyagi[1], Peyman Zirak[1], Alfons Penzkofer[1], Tilo Mathes[2], Peter Hegemann[2], Matthias Mack[3], and Sandro Ghisla[4] — [1]Institut II - Experimentelle und Angewandte Physik, Universität Regensburg, Universitätsstr. 31, 93053 Regensburg — [2]Institut für Biologie / Experimentelle Biophysik, Humboldt Universität zu Berlin, Invalidenstr. 42, 10115 Berlin — [3]Institut für Technische Mikrobiologie, Hochschule Mannheim, Paul-Wittsack-Str. 10, 68163 Mannheim — [4]Universität Konstanz, Fakultät für Biologie, Postfach 5560 M644, 78457 Konstanz

The flavin dye 8-amino-8-demethyl-D-riboflavin (AF) in the solvents water, DMSO, and methanol was studied by absorption and fluorescence spectroscopy. The first absorption band is red-shifted compared to riboflavin, and blue-shifted compared to roseoflavin. The fluorescence quantum yields are 0.22 for AF in water, 0.37 for AF in methanol, and 0.50 for AF in DMSO. The fluorescence lifetimes were found to be 2.3 ns in water, 4.9 ns in methanol, and 5.1 ns in DMSO. The non-radiative decay is thought to be dominated by internal conversion and intersystem crossing. The photo-stability of AF was studied by prolonged light exposure. For blue-light exposure (425-500 nm) quantum yields of photo-degradations were determined to be 0.000018 for AF in water and methanol, and 0.000089 for AF in DMSO. The main degradation product of AF was found to be 8-amino-lumichrome (AL, absorption rise in 310-380 nm region). AF in DMSO additionally degraded to 8-aminoflavin quinine-methide tautomer.

CPP 7: Electronic and Optical Properties of Organic Systems II

Time: Monday 14:00–16:30 Location: H39

CPP 7.1 Mon 14:00 H39

Controlling the optical properties of single molecules by optical confinement in a tunable microresonator — •Alexey Chizhik, Raphael Gutbrod, Anna Chizhik, Sebastian Baer, and Alfred Meixner — Institute of Physical and Theoretical Chemistry, University of Tuebingen, Auf der Morgenstelle 8, 72076 Tuebingen, Germany

We present experimental results on changing the fluorescence spectrum of a single dye molecule by embedding it within a tunable optical microresonator with subwavelength spacing. The resonator length is reversibly changed across the entire visible range with nanometer precision by using a piezoelectric actuator. By varying its length, the local mode structure of the electromagnetic field is changed together with the radiative coupling of the emitting molecule to the field. Since mode structure and coupling are both frequency dependent, this leads to a renormalization of the emission spectrum of the molecule. Moreover, we demonstrate how one can modify the ratio between the on- and off-axis photo emission of the molecules in the cavity. In addition, we use cylindrical vector laser beams (also known as doughnut laser modes) in the tunable microcavity to determine the longitudinal position of an isotropic emitter. By analyzing the excitation patterns resulting from the illumination of a single fluorescent bead in the focus of a radially polarized doughnut mode laser beam we can determine the longitudinal position of this bead in the microcavity with an accuracy of a few nanometers.

CPP 7.2 Mon 14:15 H39

Time resolved 3D orientation spectroscopy - experimental realisation and simulation — •Richard Börner[1], Danny Kowerko[2], Christian von Borczyskowski[2], and Christian G. Hübner[1] — [1]Institute of Physics, University of Lübeck, 23538 Lübeck, Germany — [2]Center for Nanostructured Materials and Analysis, Chemnitz University of Technology, 09107 Chemnitz, Germany

Confocal microscopy is a powerful tool for single molecule investigation of fluorescent macromolecules. Besides the common studied features in single molecule detection, the 3D orientation determination of the emission dipole enables the analysis of different conformational states. These conformational states can be represented as state depending dipole orientations intrinsic to the fluorescent molecule and/or in relation to the molecular frame. Furthermore, conformational states can be subject to intramolecular dynamics which may lead to spectral diffusion, fluorescence intensity and/or lifetime fluctuations and changes in the orientation of the emission dipole. Therefore, a simultaneous measurement of all parameters is mandatory. To this end, we show a detection scheme that allows for simultaneous determination of the full 3D emission dipole orientation, fluorescence intensity, the fluorescence lifetime and the emission spectra of single fluorescent molecules. We demonstrate the feasibility of our approach using pyridyl functionalized perylene bisimide (PBI). Moreover, monte-carlo simulations demonstrate the full potential of our detection scheme to quantify rotational dynamics on different time scales, in particular under confinement conditions.

CPP 7.3 Mon 14:30 H39

Refined determination of anisotropic dielectric tensor of α-PTCDA in the visible — Maria Isabel Alonso[1], Miquel Garriga[1], Josep Oriol Osso[2], Frank Schreiber[3], Linus Gisslen[4], and •Reinhard Scholz[4] — [1]Institut de Ciència de Materials de Barcelona, CSIC — [2]MATGAS, Campus de la Universitat Autònoma Barcelona — [3]Institut für Angewandte Physik, Universität Tübingen — [4]Walter Schottky Institut, Technische Universität München

Spectroscopic ellipsometry measurements obtained on the (102) surface of α-PTCDA are analysed with an improved scheme for the propagation of the electromagnetic wave through the monoclinic crystal [1,2]. In this approach, the exact ellipsometric equations are solved numerically within a 4×4 transfer matrix algorithm. The resulting dielectric tensor shows a pronounced anisotropy in the plane defined by the molecular transition dipoles oriented along the long axes of the two basis molecules in the unit cell, revealing a Davydov splitting of about 0.03 eV between the lowest subbands contributing to the optical response. The experimental findings are interpreted with an exciton model accounting for Frenkel excitons and charge transfer states along the stacking direction, corroborating previous assignments of the charge transfer state below neutral molecular excitations [3].

[1] M. I. Alonso, M. Garriga, N. Karl, J. O. Ossó, and F. Schreiber, Org. Electron. **3**, 23 (2002).

[2] M. I. Alonso and M. Garriga, Thin Solid Films **455-456**, 124 (2004).

[3] L. Gisslén and R. Scholz, Phys. Rev. B **80**, 115309 (2009).

CPP 7.4 Mon 14:45 H39

Visualization of a Zn(II) coordination polymer and a trinuclear Cu(II) complex by STM/CITS — •U. Mitra[1], M. Stocker[1], V. Dremov[1], N. Fischer[2], F. W. Heinemann[2], A. Zharkouskaya[3], N. Burzlaff[2], W. Plass[3], and P. Müller[1] — [1]Department of Physics and Interdisciplinary Centre for Molecular Materials (ICMM), University of Erlangen-Nürnberg, Germany. — [2]Inorganic Chemistry, Department of Chemistry and Pharmacy, University of Erlangen-Nürnberg, Germany. — [3]Institut für Anorganische und Allgemeine Chemie, Universität Jena, Germany

Topographic measurements and current imaging tunneling spectroscopy (CITS) were performed on a Zn(II) coordination polymer $[\mathrm{Zn(L)Cl}]_n$ (L = deprotonated bis(N-methylimidazol-2-ylmethyl) acetic acid) and on a trinuclear Cu(II) complex based on triaminoguanidin ($[\mathrm{Cu_3(bipy)_3(^{H}TAG)}](\mathrm{ClO_4})$). 10^{-9} molar solutions of the materials were deposited onto HOPG. In the case of the Zn(II) coordination polymer, strands of different thickness were observed. Molecular chains consisting of more than one molecule as well as clusters were also visualized for the trinuclear Cu(II) complex. In the CITS measurement, a very large current contrast was observed on the expected location of the Zn(II) and the Cu(II) metal centers. In this sense, we were able to map the internal coordination of the metal centers.

CPP 7.5 Mon 15:00 H39

Excitation Energy Transfer in Pheophorbide-a Complexes: A Mixed Quantum Classical Computation — •Jörg Megow, Zheng-wang Qu, Thomas Ronneberg, Beate Röder, and Volkhard May — Institut für Physik, Humboldt-Universität zu Berlin

The excitation energy transfer in a chromophore complex dissolved in ethanol is computed utilizing a mixed quantum classical methodology. The complex is formed by a butanediamine dendrimer to which four pheophorbide-a molecules are covalently linked. While all nuclear coordinates are described classically by carrying out room-temperature MD-simulations the electronic excitations are treated quantum mechanically utilizing a Frenkel-exciton model. A new approach is introduced to directly include intramolecular vibrations from MD-simulations into the former mixed quantum classical technique. Making a harmonic approximation to the single atom positions in respect of the so called reference structure atom positions a highly fluctuating energy was calculated and added to the chromophore complex Hamiltonian. This approach was used to further improve the existing calculations of excitation energy transfer, linear absorbance and time- and frequency resolved emission spectra, where the intramolecular vibrations were implemented parametrical only.

CPP 7.6 Mon 15:15 H39

On the chain-length dependence of Förster energy transfer for conjugated oligomers — •Rodrigo Queiroz de Albuquerque and Anna Köhler — University of Bayreuth, Physics Department, Universitätsstr. 30, 95440 Bayreuth, Germany.

Energy transfer systems comprising donor-acceptor molecules have been succesfully described using the Förster theory, which uses the Point-Dipole Approximation, PDA. However, for organic semiconductors containing extended chromophores rather small donor-acceptor distances are frequently found, and the PDA is well known to fail in correctly describing the energy transfer process. Here we report a combined experimental and theoretical study of energy transfer systems containing oligofluorenes with different conjugated chain lengths as donors and an anthracene derivative as acceptor. Blends with different amounts of donor and acceptor are investigated by means of steady-state and time-resolved spectroscopy, and the PDA is used to calculate energy transfer parameters. Our aim is also to examine the validity of the PDA in the present case, as well as to discuss the influence of the conjugated chain length of the oligofluorenes on the photophysics of the donor-acceptor systems described here.

CPP 7.7 Mon 15:30 H39

Visualizing the spin states of surface deposited Fe(II) spin-crossover compounds — •M. Stocker[1], M. S. Alam[1], A. Volkov[1], U. Mitra[1], K. Gieb[1], M. Haryono[2], K. Student[2], A. Grohmann[2], V. Dremov[1], and P. Müller[1] — [1]Department of Physics and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Germany. — [2]Institut für Chemie, Technische Universität Berlin, Germany.

We present a novel method for determining the spin states of individual molecules and small clusters of surface deposited Fe(II) spin crossover (SCO) compounds by STM. Here we focus on $[Fe^{II}(L)_2](BF_4)_2$ (L=2,6-di(1H-pyrazol-1-yl)-4-(thiocyanatomethyl)pyridine)[1]. For comparison, a high spin (HS) compound with a similar coordination motif was investigated. 10^{-8} molar solutions of the materials were drop-coated onto HOPG substrates and investigated by STM and CITS. A strong contrast between two distinct states of the SCO compound was found in the conductivity map, whereas the HS reference molecules always showed the same contrast. Therefore, the two different states can be identified with the high spin and low spin states. Switching of the spin state from high- to low-spin state and vice versa were observed at room temperature. Indications for a widening of the spin transition were found by varying the temperature.[2]

[1] M. Haryono, et al., Eur. J. Inorg. Chem. 2009, 2136.

[2] M.S. Alam, et al., Angew. Chem. (2009) (accepted).

CPP 7.8 Mon 15:45 H39

Conjugated Polymers and Fullerenes Under Oxygen Exposure: An Electron Spin Resonance Study — •Hannes Kraus[1], Andreas Sperlich[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, Div. Functional Materials for Energy Technology, D-97074 Würzburg

For applications in polymer bulk heterojunction solar cells, the blend of the polythiophene P3HT and the fullerene electron acceptor material PCBM is one of the most promising model systems until now. On the way to industrial scale processing of solar cells from these materials, the stability issue and thus the understanding of degradation mechanisms due to environmental conditions is crucial. We study the light-induced creation of polymer:oxygen-charge transfer complexes in air-exposed P3HT with electron spin resonance, and simultaneously record the evolution of the photoluminescence quenching. We identify two separate photochemical processes leading to these results, and corroborate our findings with triplet-sensitive optically detected magnetic resonance (ODMR) measurements. Furthermore, we propose a protective effect of PCBM on P3HT through triplet quenching in organic solar cells.

CPP 7.9 Mon 16:00 H39

PDMS-enclosed Liquid Crystal Lasers for Lab-On-Chip Applications — •Jürgen Schmidtke and Eugene M. Terentjev — Cavendish Laboratory, University of Cambridge, UK

During the past decade, self-assembled photonic band edge lasers based on cholesteric liquid crystals have attracted considerable interest as microscopic, coherent light sources. We demonstrate the operation of such a laser confined between optically clear and elastic polydimethylsiloxane (PDMS) rubber substrates. The formation of a planar helical texture in the cholesteric film was supported by microstructuring of PDMS layer surface, using the nano-embossing technique with glass substrates coated with conventional alignment layers as a template. With PDMS being the standard material for the fabrication of microfluidic devices, this opens a simple and flexible route for the integration of microscopic laser sources for lab-on-chip applications like spectroscopy, photo-chemistry or fluorescence cytometry.

CPP 7.10 Mon 16:15 H39

The Spectral diffusion in poly(para-phenylene)-type polymers with different energetic disorder — •Sebastian T. Hoffmann[1], Heinz Bässler[2], Jan-Moritz Koenen[3], Michael Forster[3], Ullrich Scherf[3], Ester Scheler[4], Peter Strohriegl[4], and Anna Köhler[1] — [1]Dept. of Physics, Univ. of Bayreuth — [2]Physical Chemistry, Philipps-Univ. Marburg — [3]Macromol. Chemistry, Bergische Univ. Wuppertal — [4]Dept. of Chemistry, Univ. of Bayreuth

We have employed quasi continuous fluorescence and phosphorescence spectroscopy within a temperature range between 10K and 500K to monitor the spectral diffusion of singlet and triplet excitons in a series of pi-conjugated polymers. We investigated (i) how spectral diffusion is controlled by the degree of energetic disorder present in the amorphous film, and (ii) how this process depends on the range of the electronic coupling. For singlets, and for triplets in low-disorder compounds, spectral diffusion results in a bathochromic shift of the fluorescence spectra upon cooling, until saturation sets in. In contrast, for triplets in systems with at least moderate disorder, spectral diffusion is kinetically frustrated, i.e. frozen-out.[1] This is evident through a hypsochromic shift of the phosphorescence spectra upon cooling below a characteristic temperature. The frustration effect is controlled by the jump distance, and thus it is specific for triplet excitations that migrate via short range coupling among strongly localized states as compared to singlet excitons.

[1] S.T. Hoffmann et al, Phys. Rev. B, submitted.

CPP 8: Crystallization and Self Assembly I

Time: Monday 11:00–12:45 Location: H48

Topical Talk CPP 8.1 Mon 11:00 H48

Mesoscopic structure formation of polymers in cylindrical nanopores — •Martin Steinhart — Institut für Chemie, Universität Osnabrück

Mesoscopic structure formation processes in the one-dimensional confinement of thin-film configurations, such as crystallization of semicrystalline polymers and microphase separation of block copolymers (BCPs), have been studied intensively. Only recently, the study of polymers in real two-dimensional confinement, as it is imposed by cylindrical nanopores with rigid pore walls, has emerged as a focus of interest in polymer science. Even though gaining predictive understanding as to how two-dimensional confinement modifies structure formation is still challenging, it has already become clear that inside cylindrical nanopores unprecedented mesoscopic architectures with potentially novel functionalities are accessible. As examples in case crystallization of polymers in aligned ensembles of nanopores and the self-assembly of block copolymers will be discussed. Depending on the nucleation mechanism, crystallization may result in macroscopically uniform textures. It is straightforward that polymers confined to nanoporous hosts could be ideal model systems to study polymorphism, interphases and early stages of crystallization. BCPs confined to nanopores have been found to self-assemble into unprecedented nanoscopic domain structures characterized, for example, by helical structure motifs. Studying polymeric materials in cylindrical nanopores might reveal insight into structure formation processes in general and may pave the way for new functional components made of polymeric materials.

CPP 8.2 Mon 11:30 H48

Freezing kinetics in linear pores with disorder — •Daria Kondrashova and Rustem Valiullin — Department of Interface Physics, University of Leipzig, Leipzig, Germany

Recent progress in the synthesis of nanoporous materials with controlled structural properties made it possible to address various phenomena occurring in mesoscalic molecular systems. Among them, different aspects of fluid phase transitions could now be related to the structural properties of mesoporous matrices. In this work, we take advantage of the option to prepare mesoporous silicon with linear, tailor-made pores [1] and thus to study the process of freezing of a fluid under well-defined conditions of confinement. The kinetics of this process measured in the material under study are found to be anomalously slow. We suggest a simple thermodynamical model capturing the main features observed in the experiments. In particular, we show that this behavior results from mesoscalic disorder in the pore structure, which leads to a broad distribution of local transition rates [2].

1. Khokhlov A. et al., New J. Phys. 9, 272 (2007).
2. Dvoyashkin, M., A. Khokhlov, R. Valiullin and J. Kärger, J. Chem. Phys. 129, 154702 (2008).

CPP 8.3 Mon 11:45 H48

Gyroid-structured materials via self-assembled copolymer templates — •Maik Scherer[1], Pedro Cunha[1], Alex Finnemore[1], Edward Crossland[2], and Ullrich Steiner[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge, UK — [2]Albert-Ludwigs-Universität Freiburg, Freiburg, Germany

This talk will discuss the nanostructuring of inorganic materials such as titania or single-crystalline calcium carbonate, using porous diblock copolymer thin films with gyroid morphology.

A particularly interesting phase morphology in microphase separated diblock copolymers is the so called double gyroid, where each of the immiscible blocks forms a triply periodic, self-supporting and continuous network or matrix. Together with its high surface area, the gyroid seems to be the perfect three dimensional structure for novel nanodevices.

I will present two approaches for the fabrication of gyroidal thin films employing either thermal annealing of pure PFS-b-PLA polymer or solvent annealing of a binary blend of hPS/PS-b-PI. The removal of one of the polymeric phases yields nanoporous templates. Finally, two examples for the application of these porous films as templates for inorganic materials will be presented: Firstly, the bioinspired nanostructuring of single-crystalline calcite with feature sizes as small as 37 nm. Secondly, the electrochemical deposition of titanium dioxide within the porous polymer films on a transparent, conducting substrate for high efficiency dye-sensitized solar cells.

CPP 8.4 Mon 12:00 H48

Small Angle X-Ray Scattering Study of Thermodynamic and Conformational Changes in Ion-Containing Symmetric Diblock Copolymers — •Ilja Gunkel[1,2] and Thomas Thurn-Albrecht[2] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Institute of Physics, Martin Luther University Halle Wittenberg, Halle, Germany

We present temperature-dependent SAXS measurements on two different symmetric block copolymers with added salt (Lithiumtriflate, $\mathrm{LiCF_3SO_3}$). For both studied systems, Polystyrene-b-Poly-2-vinylpyridine (PS-b-P2VP) and Polystyrene-b-Polyethyleneoxide (PS-b-PEO), the salt selectively dissolved in one block leading to large increases of the order-disorder transition temperatures ($\mathrm{T_{ODT}}$). In addition, the lamellar thickness of these ion-containing block copolymers nontrivially changed above a certain salt concentration - in PS-b-P2VP the lamellae became thicker whereas their thickness decreased in PS-b-PEO. Using basic arguments of the thermodynamics of block copolymers we were able to separate the ion-induced increase of $\mathrm{T_{ODT}}$ due to a higher incompatibility between the different blocks from changes in the thickness of the lamellae at $\mathrm{T_{ODT}}$ resulting from changes in the conformation of the ion-containing blocks.

CPP 8.5 Mon 12:15 H48

Arrays of Core-Shell Nanorods from ABC Triblock Copolymers — •Marcus Böhme[1], Bhanu Nandan[1], Manfred Stamm[1], Markus Gallei[2], and Matthias Rehahn[2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden — [2]Technische Universität Darmstadt, Ernst-Behrl-Institut, Petersenstr. 22, 64287 Darmstadt

Recently Poly-(styrene-b-ferrocenylsilane-b-2-vinylpyridine) (PS-b-PFS-b-P2VP) triblock copolymers have been reported to form core-shell like cylinders under certain solvent annealing conditions in thin films via microphase separation[1]. Here, we present our studies on structure formation in a similar polymer when applying thermal annealing using SAXS, GISAXS and SEM. Furthermore, we present our efforts to transfer the obtained structure into isolated core-shell nanorods by dissolving the matrix polymer in a selective solvent. [1] V. P. Chuang, C. A. Ross, J. Gwyther, I. Manners, Adv. Mater. 21 (37), 3789-3793, (2009)

CPP 8.6 Mon 12:30 H48

Structure formation of triphilic block copolymers micelles in water — Karsten Busse, Samuel Kyeremateng, and •Jörg Kressler — Nat.Fak. II, Institut für Chemie, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale)

The micelle formation in water of a new type of triphilic block copolymers [1] (hydrophilic poly(glycero monomethacrylate) PGMA + hydrophobic poly(propylene oxide) PPO + fluorophilic fluorodecyl F) in different compositions like ABC or CABAC structure was investigated by light and Neutron scattering.[2] The hydrophobicity of the PPO part is temperature and molecular weight dependent. The micellar structure depends on the composition of the block copolymer and temperature, and different behaviors can be observed. Due to the temperature dependence of the solubility of the PPO block in water, a collapse of the PPO should appear during heating within the observed temperature range between 5 and 60 °C. This should lead to a shrinking of the core. Depending on the length of the hydrophilic part, the shell can increase in size, due to better solubility. The aggregation behavior of two pentablock copolymers with different hydrophilic amount have been investigated in more detail by NMR, AFM, and TEM.[3]

References 1. Kyeremateng, S. O.; Amado, E.; Blume, A.; Kressler, J. Macromol. Rapid Commun. 2008, 29, 1140. 2. Kyeremateng, S. O.;Busse, K.; Kressler, J. in preparation 3. Kyeremateng, S. O.; Kressler, J. in preparation

CPP 9: Crystallization and Self Assembly II

Time: Monday 14:00–16:30 Location: H48

CPP 9.1 Mon 14:00 H48

A multi relaxation time lattice Boltzmann model for amphiphilic fluid mixtures — •Sebastian Schmieschek[1] and Jens Harting[2,1] — [1]ICP Univ Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart, Germany — [2]MTP, Dept Appl Phys, TU Eindhoven, P.O.B. 513, 5600 MB Eindhoven, The Netherlands

Due to its inherent mesoscopic character and ease of implementation and parallelisation, the lattice Boltzmann method (LBM) has become a popular model for simulations of soft matter systems. However, the broadly used single relaxation time schemes suffer from restrictions, such as a fixed Prandtl number and limited numerical stability. The introduction of a multiple relaxation time model allows a differentiated treatment of the modelled physical properties overcoming part of these problems. The present work integrates a multi relaxation time (MRT) scheme to an implementation of the popular Shan Chen type LBM. The code allows the simulation of binary and ternary multicomponent systems, containing (im)miscible and optionally amphiphilic fluid species. It has been applied to study various problems like the rheology of mesophases and microemulsions or multiphase flows in microfluidic systems. Exemplary simulations of amphiphilic mixtures and basic benchmark results of the MRT scheme are presented.

CPP 9.2 Mon 14:15 H48

Testing the Renormalized One-Loop Theory for S(q) in Diblock Copolymers — •David Morse[1,2] and Jian Qin[1] — [1]University of Minnesota — [2]University of Goettingen

We compare predictions of the renormalized one-loop (ROL) theory of correlations in block copolymers to extensive simulations of a simple bead spring model. The ROL theory is a rigorous theory of corrections to the random-phase approximation for the structure factor $S(q)$, to first order in an expansion in $N^{-1/2}$. ROL theory includes the Fredrickson-Helfand FH theory as a limiting case, in the limit of large peak-intensity, very near the ordering transition. ROL theory (but not FH theory) is found to give accurate predictions for both the peak intensity and peak wavenumber over a wide range of values of the Flory-Huggins interaction parameter χ, from $\chi = 0$ to the transition.

CPP 9.3 Mon 14:30 H48

3d versus 2d Freezing of Lennard-Jones Fluid in a Slit Pore — •Nadezhda Gribova, Axel Arnold, and Christian Holm — ICP, Universität Stuttgart

We present a computer simulation study of a (6,12)-Lennard-Jones fluid confined to a slit pore, formed by two structureless planes. These interact via a (3,9)-Lennard-Jones potential with the fluid particles. Walls in the system induce layering. In order to investigate the nature of the freezing transition, we perform a detailed analysis of the bond-orientational order parameter and diffusion in the layers. Varying the distance between the slit walls, we study the system accommodating from 1 to 7 layers. With increasing number of layers the behaviour changes from a quasi-2d crystallization without hysteresis and an intermediate hexatic phase to a standard 3d.

CPP 9.4 Mon 14:45 H48

Molecular Dynamics Simulations of Polymer Crystallization via Self-seeding — •Chuanfu Luo and Jens-Uwe Sommer — Leibniz Institute of Polymer Research Dresden, 01069, Dresden

We use large scale molecular dynamics (MD) to simulate the processes of polymer crystallization with a coarse-grained model. In total we are able to simulate 1000 polymer chains made of 1000 monomers each, a system large enough to compare to experimental relevant, entangled melts. It is found that some micro crystalline domains (MCDs) can survive slightly above the apparent melting temperature after a cooling and reheating cycle. We chose the stablest MCD as a baby seed and let it grow at a constant quenched temperature. A single lamella can be formed via this self-seeding process. We observe the growth pathway and analyze the chain dynamics especially at the growth front. We thank the financial support by Deutsche Forschungsgemeinschaft (DFG) SO 277/6-1.

Selected references: [1] C. Luo and J. Sommer, Comp Phys. Comm. 180, 1382 (2009) [2] C. Luo and J. Sommer, Phys. Rev. Lett. 102, 147801 (2009) [3] J-J. Xu, Y. Ma, W.B. Hu, M. Rehahn and G. Reiter, Nature Materials 8, 348 (2009)

CPP 9.5 Mon 15:00 H48

Novel method for the growth of highly crystalline P3HT thin films — •Shabi Thankaraj Salammal[1], Martin Brinkmann[2], Patrick Pingel[3], Ullrich Pietsch[1], Nils Koenen[4], and Ullrich Scherf[4] — [1]Solid State Physics, University of Siegen — [2]Institute Charles Sadron, Strasbourg. — [3]Soft Matter Physics, University of Potsdam. — [4]Macromolecular Chemistry, University of Wuppertal.

Role of growth temperature in crystallinity of P3HT thin films have been demonstrated here. Films were prepared at RT and -30°C above the OTS treated SiO2 substrate. X-ray diffracted intensity of -30°C grown film gained by the factor of 3 while comparing the films prepared on with and without OTS treated substrates. The degree of preferential orientation has been quantified via Chi scan, where incident and detector angle were fixed under specular condition of (100) Bragg peak. The OTS treated substrate provides a higher number of oriented crystallites than the non OTS treated one; it could be due to the possible interdigitation of OTS and P3HT polymer side chains. Diffracted intensity of -30°C grown film has one order of magnitude higher than the RT grown one. 2D x-ray diffraction pattern envisage the presence of flat and edge-on-orientation in RT grown film but flat-on-orientation is completely absent at -30°C casted one. X-ray diffraction has been confirmed by electron diffraction as well. HRTEM image envisage the presence of flat-on orientation in spin coated film. The luminescence intensity gained by the factor of two and mobility gained by one order of magnitude while comparing -30°C casted with RT, those results will be correlated with increase in conjugation length of the polymer.

CPP 9.6 Mon 15:15 H48

What controls heterogeneous nucleation of polymers at interfaces? — •Thomas Henze, Klaus Schröter, and Thomas Thurn-Albrecht — Martin-Luther-University Halle-Wittenberg, Institute of physics, D-06199 Halle (Saale), Germany

We here present a study of the morphology of thin films of polyethylene crystallized from melt on a number of substrates with different ability to invoke crystallization, namely mica, NaCl, SiO_2 and HOPG. Using intermittent-contact mode AFM very different structures are observed on the surface of the polymer films depending on the kind of substrate, the film thickness as well as the degree of branching of the polymer.

For very thin films (about 30 nm) on NaCl and HOPG short, edge-on lamellae oriented according to the symmetry of the underlying crystal lattice show up indicating epitaxial growth. With increasing film thickness (up to 300 nm) the preferred edge-on orientation of the lamellae remains, while the in-plane orientation tends towards one fixed direction. The morphology itself indicates a very high nucleation ability for these kind of substrates. In contrast to that on SiO_2 and mica a spherulitic structure is present showing a preferred flat-on orientation of the lamellae in the thinnest films. However, a quantitative analysis of nucleation density shows that also on these substrates heterogeneous, but non-epitaxial nucleation takes place.

CPP 9.7 Mon 15:30 H48

Local and Collective Motions in Polyolefins with Precise Alkyl Branches: a Solid State NMR Study — •Robert Graf[1], Yuying Wei[2], Kenneth B. Wagener[2], and Hans Wolfgang Spiess[1] — [1]Max-Planck-Institut für Polymerforschung, Mainz, Germany — [2]University of Florida,Gainesville, Florida (USA)

In linear polymers, such as polyethylene (PE), chain branches change the local mobility and have pronounced effects on the mechanical properties, such as processablity and drawability. In many previous studies, the irregular distribution of the branching sites along the main chain caused an uncertainty of the branching influence on morphology, chain dynamics, as well as other physical properties. Here results from investigations of dynamic processes in crystalline regions of PE samples with regular spaced methyl branches. By deuteration of the methyl branches, the molecular dynamics of the defect site can be studied selectively via 2H NMR methods, whereas molecular reorientations of the polymer chain between the branching sites can be monitored separately via 13C chemical shift anisotropy measurements. Combining these results with studies of local conformations, a twist motion can be identified, which is localized at the branching sites for a spacing of more than twenty CH2 units between subsequent branching points. In methyl branched PE samples with shorter spacing, a collective dynamic process can emerge from this twist motion, which ultimately leads to the formation of a rotator phase.

CPP 9.8 Mon 15:45 H48

Single-Molecule Force Spectroscopy of Supramolecular Heterodimeric Capsules. — •Tobias Schröder[1,2], Thomas Geisler[2], Björn Schnatwinkel[2], Dario Anselmetti[1], and Jochen Mattay[2] — [1]Department of Physics, Experimental Biophysics & Applied Nanosciences, Bielefeld University, — [2]Department of Chemistry, Organic Chemistry I, Universitätsstrasse 25, 33615 Bielefeld, Germany

Despite the rich information accessible, atomic-force single-molecule force spectroscopy (AFM-SMFS) has scarcely been employed to analyze the bonding between building blocks of complex supramolecular structures [1]. After the pioneering work by Eckel et al. [2], we investigated the multiple bonding interaction in a supramolecular capsule held together by four hydrogen bonds [3]. The measured dissociation forces of the heterodimeric capsule represent the mechanical stability of the supramolecular system and allow a quantitative evaluation of the interaction yielding the kinetic dissociation rate constant k(off), the reaction length $x(\beta)$ and the standard Gibbs free energy $\Delta G0$ according to the Bell-Kramers model.

[1] M. Janke, Y. Rudzevich, O. Molokanova, T. Metzroth, I. Mey, G. Diezemann, P. E. Marszalek, J. Gauss, V. Böhmer, A. Janshoff, Nat. Nanotechnol. 2009, 4, 225-229.

[2] C. Schäfer, R. Eckel, R. Ros, J. Mattay, D. Anselmetti, J. Am. Chem. Soc. 2007, 129, 1488-1489.

[3] T. Schröder, T. Geisler, B. Schnatwinkel, D. Anselmetti, J. Mattay, submitted.

CPP 9.9 Mon 16:00 H48

Temperature dependent changes in the mechanism of plastic deformation of Polypropylene — •Konrad Schneider and Andreas Schöne — Leibniz-Institut für Polymerforschung Dresden, Hohe Str. 6, 01060 Dresden, Germany

The mechanical behaviour of semi-crystalline polymers is dependent on the mechanical behaviour of the crystalline and the amorphous phase as well as their interaction. All those are temperature dependent. Online-WAXS and -SAXS enables to monitor strain dependent the changes within the different phases during deformation and fracture. For the example of Polypropylene it will be demonstrated how the initial lamellae break down into crystalline blocks which disappear in oriented stands in the case of cold drawing, accompanied by cavitation. At higher temperatures the crystalline blocks remain stable and become arranged between fibrilar crystals.

CPP 9.10 Mon 16:15 H48

Robobeads: towards remote friction measurements at small scales — •Stephan Herminghaus[1], Zeina Khan[1], Audrey

Steinberger[1], and Ralf Seemann[2] — [1]MPI für Dynamik und Selbstorganisation, Göttingen — [2]Universität des Saarlandes, Fakultät für Physik

We have recently discovered that small adhesive spheres may assemble to form aggregates which perform rapid locomotion on a substrate if an external oscillatory drive field is applied. The concept is demonstrated with sub-millimetric wet spheres on a horizontally vibrated flat plate. Quite strikingly, the aggregates tend to align by themselves such as to extract the maximum energy from the drive field. A theoretical treatment shows that this concept is quite robust and under certain circumstances may be scalable down to the sub-micron range

CPP 10: Poster: Structure and Dynamics of Responsive Hydrogels

Time: Monday 16:30–18:00 Location: Poster C

CPP 10.1 Mon 16:30 Poster C

Temperature dependent switching kinetics and aging effects of gold coated end-capped PNIPAM thin films — •Weinan Wang[1], Jan Perlich[1], Gunar Kaune[1], Achille M. Bivigou Koumba[2], Andre Laschewsky[2], Christine M. Papadakis[1], Robert Cubitt[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik - Department E13, Garching, Germany — [2]Uni. Potsdam, Inst. Chemie, Potsdam-Golm, Germany — [3]ILL, Grenoble, France

Poly(N-isopropylacrylamide) (PNIPAM) is one of the prominent thermo-sensitive hydrogels for the construction of nanoscale electric switches 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 structures of the dry films before and after switching are characterized with AFM. The internal structures after each swelling-deswelling cycle are investigated by grazing incidence small angle x-ray scattering (GISAXS). The temperature dependent switching kinetics and aging effects in water vapour of such 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 electric switches applications

CPP 10.2 Mon 16:30 Poster C

Star-PEG-Heparin-Polyelectrolyte-Hydrogels- viscoelasticity and swelling behavior — •Ron Dockhorn[1,2], Uwe Freudenberg[1], Petra B. Welzel[1], Kandice Levental[1], Jens-Uwe Sommer[1,2], and Carsten Werner[1] — [1]Leibniz Institute of Polymer Research Dresden, D-01069 Dresden, Germany — [2]Technische Universität Dresden, Institute for Theoretical Physics, D-01069 Dresden, Germany

We are studying a new class of biohybrid networks made of heparin (HEP), a highly charged glycosaminoglycan, and non-charged, elastic 4-star-shaped-polyethylene glycol (PEG) in solutions of various salt concentrations. We use a mean-field type model to understand the combined effects of counterions and a good solvent on the swelling properties of the gels. By changing the mole-fraction between HEP and PEG the effective degree of cross-linking can be controlled. The interplay between charge and excluded volume effects lead to nearly constant heparin concentration in the swollen gel under physiological conditions, independent of the mole-fraction at preparation while allowing large variations of the storage modulus and degree of swelling. This opens the possibility to synthesize gels which allow a constant release of heparin-binding signaling molecules while independently controlling the mechanical properties to optimize matrices with both mechanical and biomolecular cues for cell replacement-based therapies.

CPP 10.3 Mon 16:30 Poster C

The Self-assembly of Triblock Copolymers into Smart Hydrogels. Comparing PolyNIPAM with PolyMDEGA as Responsive Hydrophilic Block — •Anna Miasnikova[1], Achille Mayelle Bivigou-Koumba[1], André Laschewsky[1], Peter Müller-Buschbaum[2], and Christine M. Papadakis[2] — [1]Department of Chemistry, University of Potsdam — [2]Physikdepartment E13, Technische Universität München

Amphiphilic block copolymers, consisting of a hydrophilic A and a hydrophobic B block, self-assemble into a wealth of supramolecular structures. Depending on the concentration they are known to associate into micelles, followed by clusters, and finally into macroscopic hydrogels. For BAB-type triblock copolymers, the association deals with an even more complex situation. Instead of forming only core-shell micelles, an open association leading to branched structures with improved swelling properties may occur.

In this context, we are exploring symmetrical triblock copolymers of the BAB type. Copolymers were synthesised with long hydrophilic A and short styrenic B blocks that are directly soluble in water. Moreover, we implemented thermo-responsive "smart" A blocks in these block copolymers, enabling to switch the amphiphilic behaviour "on" and "off". Poly(N-isopropylacrylamide) PolyNIPAM and poly(methoxy diethylene glycol) PolyMDEGA were chosen as hydrophilic blocks with a similar lower critical solution temperature. Characteristic differences are found between the two different "smart" blocks, as studied by dynamic light scattering (DLS) and rheology.

CPP 10.4 Mon 16:30 Poster C

Collapse behavior of thermo-responsive poly(2-oxazoline) copolymers — •Christine M. Papadakis[1], Stephan Salzinger[2], Stephan Huber[2], Joseph Adelsberger[1], Anastasia Golosova[1], Andreas Meier-Koll[1], Peter Busch[3], Sandor Balog[4], and Rainer Jordan[2] — [1]TU München, Physikdepartment E13, Garching — [2]TU München, Department Chemie, Garching — [3]JCNS, FRM II, Garching — [4]PSI, Villigen, Switzerland

The poly(2-oxazoline) (POx) system offers the possibility to tune the water-solubility in a wide range. Moreover, using 2-isopropyl (iPr) as a side group results in a thermo-responsive polymer with a lower critical solution temperature (LCST) [1].

We have investigated the LCST behavior of an iPrOx homopolymers as well as a gradient copolymer with few n-nonyl-2-oxazoline (NOx) groups in aqueous solution. The LCST and the molecular aggregation behavior were studied using single molecule as well as ensemble characterization techniques (fluorescence correlation spectroscopy (FCS), turbidimetry and small-angle neutron scattering). We have found that iPrOx in aqueous solution shows mean-field temperature behavior and forms large aggregates above the LCST. In contrast, the collapse behavior of the gradient copolymer shows more complex behaviour. In addition to the large aggregates formed at the LCST, the polymers form small globules which gradually grow as temperature is increased.

[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 10.5 Mon 16:30 Poster C

Structure and dynamics of thermoresponsive blockcopolymer gels — •Joseph Adelsberger[1], Andreas Meier-Koll[1], Weinan Wang[1], Achille M. Bivigou-Koumba[2], André Laschewsky[2], Thomas Hellweg[3], Olaf Holderer[4], Vitaliy Pipich[4], Peter Busch[4], Peter Müller-Buschbaum[1], and Christine M. Papadakis[1] — [1]TU München, Physik-Department E13, Garching — [2]Universität Potsdam, Institut für Chemie — [3]Universität Bayreuth, Physikalische Chemie I — [4]Jülich Center of Neutron Science, Garching

Thermoresponsive polymer gels display strong changes in volume when heated above the lower critical solution temperature (LCST). Therefore they are interesting candidates for applications in ultrafiltration or as drug delivery systems. 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 small-angle neutron scattering (SANS) and dynamic light scattering [1]. The micellar radius shows a sudden decrease at the LCST, i.e. the formerly hydrophilic shell shrinks. Above the LCST, the collapsed micelles form clusters, and water is released. The kinetics of the collapse transition is investigated in time-resolved SANS measurements. Neutron spin-echo spectroscopy is used to study the segmental dynamics of the hydrophilic block. The intermediate scattering function displays the fast PNIPAM segmental motion and the slow micellar diffusion.

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

CPP 10.6 Mon 16:30 Poster C

Hydrogels based on NIPAM — •Marcel Richter 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.

One aim of our studies is the raise of the size of microgels which we build up to around 1 *m. In this case we follow two strategies of preparing these particles. On the one hand we use core-shell microgel with NIPAM and on the other hand we added a co-monomer into the core surrounded by a NIPAM shell. For both strategies microgel particles are synthesized by emulsion polymerization without using any surfactants at temperature about 70°C [2]. The size of microgels is determined by Dynamic Light Scattering and Atomic Force Microscopy. The prepared nanoparticles were used for investigation on silica surfaces. Here, the behaviour and the coverage of the surface are investigated by changing external parameter like temperature and salinity.

[1] *K. Kratz, T. Hellweg, W. Eimer, Polymer (2001), 42, 6531 [2]*R. Pelton, Adv. Colloid Interface Sci. (2000), 85, 1

CPP 10.7 Mon 16:30 Poster C

Thermoresponsive Behaviour of adsorbed P(NIPAM-co-AAc) Microgel Particles — Anna Burmistrova, •Marcel Richter, and Regine von Klitzing — Technische Universität Berlin, Straße des 17. Juni 124, 10623 Berlin, Germany

During the last decades microgels made of N-isopropylacrylamide (NIPAM) have attracted much interest and were studied by several techniques like microscopy and light scattering [1]. These polymer particles show thermoresponsive behaviour and can therefore be classified as *smart* materials. Monodisperse PNIPAM microgels were synthesized by emulsion polymerisation without using surfactants. To receive the pH-sensitive microgels, aclylic acid (AAc) as a co-monomer was used. [2, 3]. The particles were adsorbed on the different substrates (silicon precoated with different polyelectrolytes and gold) [4, 5]. The thermo induced swelling/deswelling behaviour of adsorbed microgels was studied by Atomic Force Microscopy and Quartz Crystal Microbalance methods. The effect of co-monomer content (AAc), effect of pH and effect of ionic strength were investigated.

[1] K. Kratz, T. Hellweg, W. Eimer, Polymer (2001) 42, 6531 [2] S. Höfl, l. 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, T. Hellweg, R.v. Klitzing, Langmuir (2008), 24, 12595 [5] Stephan Schmidt, Hubert Motschmann, Thomas Hellweg, Regine von Klitzing, Polymer (2008), 49, 3, 749

CPP 10.8 Mon 16:30 Poster C

Characterization of PMDEGA based hydrogel films — •Qi Zhong[1], Gunar Kaune[1], Monika Rawolle[1], Ezzeldin Metwalli[1], Achille M. Bivigou-Koumba[2], Andre Laschewsky[2], Christine M. Papadakis[1], Robert Cubitt[3], and Peter Müller-Buschbaum[1] — [1]Technische Universität München, Physik Department E13, James-Franck-Str.1, 85747 Garching, Germany — [2]Potsdam Universität, Inst. Chemie, Karl-Liebknecht-Str. 24-25, 14476 Potsdam-Golm, Germany — [3]Institut Laue-Langevin, 6 rue Jules Horowitz, 38000 Grenoble, France

Stimuli-sensitive hydrogels exhibit interesting properties which attract increasing attention due to a large variety of applications such as drug delivery, sensors and bioseparation. A novel thermoresponsive poly(monomethoxy diethyleneglycol acrylate) (PMDEGA) exhibits a higher lower critical solution temperature (LCST) when compared to the frequently investigated thermoresponsive polymer poly(N-isopropylacrylamide) (PNIPAM). Thus PMDEGA can be an interesting alternative to PNIPAM in tropical countries where the temperature is above the LCST of PNIPAM. In order to create an internal ordering in the thin hydrogel films of PMDEGA, the homopolymer is replaced by a PMDEGA based tri-block copolymer with polystyrene as an end group, P(S-b-MDEGA-b-S). Thin films of homo- and tri-block polymer with different thickness are prepared by spin coating and characterized with X-ray reflectivity and white light interferometry. Neutron reflectivity is used to investigate the kinetic behaviour of the films in temperature jumps above LCST.

CPP 10.9 Mon 16:30 Poster C

Environment-friendly photolithography using poly-(N-isopropylacrylamide)-based thermoresponsive photoresists — •Leonid Ionov[1], Nikolay Puretskiy[1], Georgi Stoychev[1], Svetlana Zakharchenko[1], Stefan Diez[2], and Manfred Stamm[1] — [1]Leibniz-Institut fuer Polymerforschung Dresden e.V., Dresden, Germany — [2]Max-Planck-Institute of Molecular Cell Biology and Genetics, Dresden, Germany

We report a novel approach for the temperature-triggered development of water-soluble photoresists based on photocleavable poly-(N-isopropylacrylamide) copolymers. These copolymers are soluble in aqueous environment below their Lower Critical Solution Temperature (LCST). Upon UV irradiation, the photocleavable groups are deprotected resulting in an increased LCST. Thus, the illuminated parts of spin-coated copolymer layers dissolve at higher temperatures than the surrounding areas, leading to pattern development. The photoresist can finally be completely removed at low temperature. We demonstrate the applicability of this novel photolithographic approach by the patterning of fluorescent proteins.

CPP 11: Poster: New Instruments and Methods

Time: Monday 16:30–18:00 Location: Poster C

CPP 11.1 Mon 16:30 Poster C

Versatile Object-oriented Toolkit for Coarse-graining Applications — Victor Rühle, •Christoph Junghans, Alexander Lukyanov, Kurt Kremer, and Denis Andrienko — Max-Planck-Institut für Polymerforschung, Ackermannweg 10, D-55128 Mainz, Germany

Coarse-graining is a systematic way of reducing the number of degrees of freedom representing a system of interest. Several coarse-graining techniques have so far been developed, such as iterative Boltzmann inversion, force-matching, and inverse Monte Carlo. However, there is no unified framework that implements these methods and allows their direct comparison. We present a versatile object-oriented toolkit for coarse-graining applications (VOTCA)[1] that implements these techniques and provides a flexible modular platform for the further development of coarse-graining techniques. All methods are illustrated and compared by coarse-graining the SPC/E water model, liquid methanol, liquid propane, and a single molecule of hexane.

[1] V. Rühle, C. Junghans, A. Lukyanov, K. Kremer, D. Andrienko, Versatile Object-oriented Toolkit for Coarse-graining Applications, J. Chem. Theo. Comp. doi: 10.1021/ct900369w (2009)

CPP 11.2 Mon 16:30 Poster C

Replacement of Density Matrix Calculations by Observable Equations — •Günter Hempel — Martin-Luther-Universität, Institut für Physik, Betty-Heimann-Str, 7, 06120 Halle

The density matrix formalism is used frequently for calculations of the time evolution of spin systems, e.g. in magnetic resonance spectroscopy. The dimension of the density matrix, however, increases strongly if the number of participating spins grows. As an example, the still small system of three protons and one carbon-13 nucleus generates a 16-dimensional Hilbert space of wave functions leading to a density matrix of 256 elements. Often symmetry relations allow to conclude that some of the elements are constant or zero, others might be linearely dependent on anothers again, but nevertheless the number of differential equations we are left with might be very large. To obtain shorter systems of differential equations a method is proposed which transforms the Liouville-von Neumann-equation into a system of differential equations of observables (instead into one of matrix elements). Generally the number of differential equations of observables is essentially smaller that that of density-element equations. Examples are given which demonstrate the handling of the method and the reduction of the system of differential equations. Applications concern the spin dynamics during polarization transfer within ensembles of spin systems as well as elementary processes of spin diffusion.

CPP 11.3 Mon 16:30 Poster C

Compact magnet array for portable high-resolution NMR and Imaging — •Ernesto Danieli, Juan Perlo, Bernhard Blümich, and Federico Casanova — ITMC, RWTH Aachen University, Worringerweg 1, D-52074,Aachen, Germany

Portable NMR probes built from permanent magnets offer several advantages over conventional NMR systems. However, the inhomogeneity of the magnetic field generated by these sensors precludes their use in high resolution NMR spectroscopy and MRI. Recently we have demonstrated that the inhomogeneities of the magnetic field can be removed by providing the sensor with movable permanent magnets which allows generating and controlling harmonic field corrections by a mechanical shimming approach [1,2]. In this work we present a high-performance magnet design based on this concept, which enables us to reduce the size of the magnet keeping the field strength and the sample volume constant. In particular, it was used to build a palm size magnet working in a volume large enough to fit conventional 5 mm NMR tubes where the high field homogeneity allowed us to measure proton NMR spectra of different solvents with a resolution better than 0.16 ppm at 30 MHz. By scaling the dimensions of the magnet the same geometry was optimized to build a portable MRI scanner for imaging samples of 4 cm DSV

1. J. Perlo, F. Casanova, and B. Blümich, Science, 315 (2007) 1110-1112.
2. E. Danieli, J. Mauler, J. Perlo, B. Blumich, and F. Casanova, J. Magn. Reson., 198 (2009) 80-87

CPP 11.4 Mon 16:30 Poster C

Simultaneous investigation of morphological characteristics and crystallinity of thin nanocomposite films — •Jan Perlich[1], Jan Rubeck[1], Peter Müller-Buschbaum[2], Stephan V. Roth[1], and Rainer Gehrke[1] — [1]HASYLAB at DESY, Hamburg — [2]TU München, Physik-Department LS E13, Garching

Thin nanocomposite films formed by polymer or colloidal templates consisting of various material systems are employed in many fields such as coatings, sensors, photovoltaics, catalysis, magnetic recording and biomimetics. The preparation techniques enable the fabrication of thin films with tailor-made morphologies and specific properties. In order to correlate the characteristics of the fabricated thin films with the employed parameter settings at preparation, a detailed characterization is necessary. The simultaneous investigation of the morphological characteristics as well as the crystallinity of thin, crystalline metal oxide films is performed by small and wide angle X-ray scattering at grazing incidence (GISAXS and GIWAXS/GIXD). The small angle scattering beamline BW4 of HASYLAB, as a dedicated materials science beamline, is most suitable for such an investigation enabling the simultaneous access to an extended scattering q-range for GIWAXS. In addition, the introduction of a sample environment with defined environmental conditions, e.g. inert gas, heating and vapor treatment, enables in-situ observations of the thin nanocomposite films regarding several questions. Recent experimental data is presented and the X-ray scattering investigation is complemented in real space by surface and thin film sensitive probes.

CPP 11.5 Mon 16:30 Poster C

Status of the micro- and nanofocus x-ray scattering beamline at PETRA III — •Stephan V. Roth[1], Mottakin M. Abul Kashem[1], Gunthard Benecke[1,2], Adeline Buffet[1], Ralph Döhrmann[1], Rainer Gehrke[1], Völker Körstgens[3], Christina Krywka[4], Jannis Lehmann[5], Martin Müller[3], Peter Müller-Buschbaum[1], Kai Stassig[1], and Edgar Weckert[1] — [1]HASLYAB at DESY, Notkestr. 85, D-22607 Hamburg — [2]MPIKG, Am Mühlenberg 1, D-14476 Potsdam — [3]IEAP, CAU, Leibnizstr. 19, D-24098 Kiel — [4]GKSS, Max-Planck-Str. 1, D-21502 Geesthacht, — [5]Physik-Department E13, TU München, James-Franck-Str. 1, D-85748 Garching

The micro- and nanofocus SAXS/WAXS beamline P03 (MiNaXS), combines micro- and nano-focused x-ray beams with small- and wide-angle x-ray scattering (SAXS/WAXS). Situated at the third generation high-brilliance source PETRA III of DESY in Hamburg, Germany, MiNaXS allows for high resolution in both real and reciprocal space with beam sizes ranging from 40μm to 100nm. The low divergence offered by the high-β-undulator allows for combining ultra-SAXS geometries with such small beams. We present the current status of commissioning of the MiNaXS beamline. Strong emphasis is put on the future improvements of the various experimental in-situ scanning techniques, such as nano- and μGISAXS [1] as well as its possible combinations with high-throughput and industrial processing methods for thin film technology and fluidics [2]. [1] Roth et al., Langmuir (2009), DOI: 10.1021/la9037414 [2] Moulin et al., Rev. Sci. Instr. 79, 015109 (2008)

CPP 11.6 Mon 16:30 Poster C

PolLux - a soft x-ray nanoprobe for soft matter studies — •Andreas Späth[1], Jörg Raabe[2], Christian Hub[1], George Tzvetkov[1,2], and Rainer Fink[1] — [1]Physical Chemistry, Univ. Erlangen, Erlangen, Germany — [2]Swiss Light Source (SLS), Paul Scherrer Institut, Villigen, Switzerland

Zone-plate based x-ray microscopes offer a wide range of potential applications in fundamental and applied science, in physics, chemistry and material science or in the imaging of biosamples. The present PolLux scanning transmission x-ray microspectroscope (PolLux-STXM) is installed at a bending magnet beamline of the Swiss Light Source (SLS) operating from 260 - 1200 eV [1]. Using the latest zone-plate technology, imaging of lateral structures with 12 nm periods was achieved [2]. The available energy range is ideally suited for soft matter investigations. We will present spectromicroscopic results from various organic based materials, like organic hybrid materials (microspheres, microballoons), polymer films, organic nanocrystals or biosamples. The recent extension of the detection setup by an electron multiplier offers additional surface-enhanced detection. Thus, we are able to combine sulk and surface sensitivity. In addition, differential phase-contrast (DPC) imaging offers another detection scheme to improve image contrast. The complementary use of the various detection schemes offers improved knowledge on the investigated soft matter samples.

The project is funded by the BMBF under contract 05 KS7WE1.

1. J. Raabe, et al., Rev. Sci. Instrum. 79, 2008, 113704.
2. K. Jefimovs, et al., Phys. Rev. Lett. 99, 2007, 264801.

CPP 11.7 Mon 16:30 Poster C

Micro total analysis system: A combination of a magnetic ratchet with giant magnetoresistance sensors — •Alexander Auge, Thomas Weiss, Dieter Akemeier, Frank Wittbracht, Alexander Weddemann, and Andreas Hütten — Uni Bielefeld, Fakultät für Physik, Universitätsstr. 25, 33615 Bielefeld, Germany

Micro Total Analysis Systems (μ TAS) on microfluidic chips is a rapidly growing field due to the large variety of possible applications like point of care diagnostics. The aim of μ TAS is to integrate all laboratory tasks on one microfluidic chip. These tasks include sample preparation, injection, manipulation, reaction, separation and detection. In this area the use of magnetic markers like beads or nanoparticles has gained importance. These markers can be selectively functionalized so that they can be attached to a variety of bioconjugates and provide reaction sites for chemical binding. One possible idea to transport, separate and detect magnetic beads is the ratchet concept. The basic idea of a ratchet is to use diffusion and a fluctuating asymmetric potential to move the magnetic markers. In this work, the ratchet is realized via a spatially periodic array of conducting lines and a magnetic out-of-plane field to create the asymmetric potential. Giant magnetoresistance sensors are placed in the potential minima of the ratchet leading to the possibility of bead detection; this allows an integrated analysis of the bead velocity. Since the bead velocity is size dependent, this enables drawing conclusions regarding e.g. bead-bacteria bindings.

CPP 11.8 Mon 16:30 Poster C

Concepts for magnetoresistive sensors and microfluidic integration — •Dieter Akemeier, Alexander Auge, Frank Wittbracht, Alexander Weddeman, and Andreas Hütten — Uni Bielefeld, Fakultät für Physik, Universitätsstr. 25, 33615

Point-of-care diagnostics is a rapidly growing field with the aim to miniaturize standard laboratory tests. Using magnetic point-of-care diagnostic devices has various advantages compared to other approaches like the direct read out of giant magneto resistance sensors, low interaction with biologic materials and low cost production.

The detection of antigens or bacteria in the continuous flow approach uses selective binding of magnetic markers on functionalized sensor surfaces located on the bottom of the flow channel. To position the particles on top of the sensor array a microfluidic structure of changing height is used. This increases the capture rate by more than 100% in comparison to a straight channel and leads to a homogeneous sensor coverage. By placing an array of 32 magnetoresistive sensors at certain position within the microfluidic system, it is possible to catch biomolecules from different starting heights on specified sensors. The experimental detection process will be discussed in detail and is compared with theoretical predictions.

CPP 11.9 Mon 16:30 Poster C

Novel techniques for the exploration of three-dimensional molecular order — •Wilhelm Kossack[1], Periklis Papadopoulos[1], Friedrich Kremer[1], Felicitas Brömmel[2], Patrick Heinze[2], and Heino Finkelmann[2] — [1]Universität Leipzig, Institut für experimentelle Physik I, Linnestr. 5, 04103 Leipzig — [2]Albert Ludwigs Universität Freiburg, Institute for Macromolecular Chemistry, Stefan Meier-Str. 31, 79104 Freiburg

Liquid Crystal Elastomers (LCE) form a novel class of materials combining the properties of liquid crystals with elastomeric networks and which can cover several application areas due to their chemical diversity. IR-Transition Moment Orientational Analysis (IR-TMOA) is employed in order to determine mean orientation and molecular order parameter of the different molecular moieties (mesogen, polymer backbone, etc.). This technique takes advantage from the specifity 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 Maxwells-equations enables one to determine seperately the spatial orientation function of each molecular group. This provides a detailled insight into the intramolecular interactions and thus into the mechanisms governing order.

CPP 11.10 Mon 16:30 Poster C

Time resolved 3D orientation spectroscopy of functionalized perylene bisimide (PBI) molecules — •Richard Börner[1], Danny Kowerko[2], Stefan Krause[2], Christian von Borczyskowski[2], and Christian G. Hübner[1] — [1]Institute of Physics, University of Lübeck, Ratzeburger Allee 160, 23538 Lübeck, Germany — [2]Center for Nanostructured Materials and Analysis, Chemnitz University of Technology, 09107 Chemnitz, Germany

Fluorescence detection on a single molecule level has been used to investigate interconversions between different molecular conformational states of perylene bisimide (PBI) type molecules, which are subject to intramolucular dynamics due to flexible bay groups [2]. This intramolecular dynamics may lead to spectral diffusion, fluorescence intensity and/or lifetime fluctuations and changes in the orientation of the emission dipole. Therefore, a simultaneous measurement of all parameters is mandatory. To this end, we show a detection scheme that allows for simultaneous determination of the full three-dimensional emission dipole orientation, fluorescence intensity, the fluorescence lifetime and the emission spectra of single fluorescent molecules. The obtained ms time resolution for the orientation determination [1] in comparison to other methods enables a simultaneous access on fast intramolecular conformational dynamics accompanied by changes in the orientation of the fluorescence emission dipole that is in the long axis of the dye PBI molecule.

[1] J. Hohlbein & C. G. Hübner, JCP, 129, 094703 (2008)
[2] D. Kowerko et al., Molecular Physics, 107 (2009)

CPP 11.11 Mon 16:30 Poster C

Local thermomechanical characterization of phase transitions on polymers using heated SFM-probes — •Thomas Fischinger, Martin Laher, and Sabine Hild — Department of Polymer Science, Johannes Kepler University Linz, Altenbergerstrasse 69, 4040 Linz, Austria

Thermal analysis methods are important instruments for polymeric research, however, up to now mainly bulk properties are detected. Local thermal analysis (LTA) based on scanning probe microscopy (SPM) allows the probing of melting and glass transition temperatures on a 100 nm length scale. To understand local mechanisms for temperature-induced phase transitions in polymers quantitative measurements of characteristic thermomechanical properties such as glass transition and melting temperatures as well as temperature dependent elastic and loss modulus and thermal expansion coefficients in nanoscale volumes are required. Since conventional LTA is insensitive to changes in the dissipative properties in the materials a new approach based on the combination of acoustic atomic force microscopy band excitation detection and a heated tip probe is for the unambiguous detection of changes in resonance frequency and tip-surface dissipation. In the first step, an appropriate temperature calibration method has been established using carboxylic acids with defined melting points to correlate the deflection signal or amplitude and frequency changes with the temperature of the probe. Bases on this, the glass transition temperature will be determined on microscopic scale. The opportunities given by this method are demonstrated in selected model polymeric systems.

CPP 12: Poster: Electronic and Optical Properties of Organic Systems

Time: Monday 16:30–18:00 Location: Poster C

CPP 12.1 Mon 16:30 Poster C

Photo-Induced Phase Changes in Azobenzene-Containing Materials — •Hubert Audorff[1], Lothar Kador[1], Roland Walker[2], and Hans-Werner Schmidt[2] — [1]University of Bayreuth, Institute of Physics and BIMF, D-95440 Bayreuth, Germany — [2]University of Bayreuth, Macromolecular Chemistry I and BIMF, D-95440 Bayreuth, Germany

The photo-induced formation of liquid-crystalline phases in azobenzene-containing amorphous materials is demonstrated. Liquid-crystalline polymers and low-molecular-weight glass formers can be quenched into a stable amorphous phase at room temperature. During the inscription of holographic intensity gratings, the illuminated areas become liquid-crystalline, which stabilizes the orientation of the azobenzene units, leading to stable gratings. Another advantage of the quenched polymeric materials is that the writing times are shorter by several orders of magnitude as compared to liquid-crystalline azobenzene compounds. With a series of low-molecular-weight tris-azobenzene derivatives, a remarkably stable light-induced orientation of the chromophores in initially amorphous thin-film architectures is demonstrated for the first time. The liquid-crystalline character is caused by spacers between the tris-functionalized benzene core and the three azobenzene moieties as well as polar end groups. The formation of the liquid-crystalline phase manifests itself in a pronounced post-development of the inscribed ratings, *i. e.*, an increase of the diffraction efficiency after the end of the writing process.

CPP 12.2 Mon 16:30 Poster C

Frequency-Domain FLIM Measurements of Fluorophore Mixtures with a Custom-Built Low-Cost Setup — •Thomas Bezold and Lothar Kador — University of Bayreuth, Institute of Physics and Bayreuther Institut für Makromolekülforschung (BIMF), 95440 Bayreuth, Germany

Fluorescence lifetime imaging microscopy (FLIM) in the frequency domain is applied to different binary mixtures of fluorophores. The custom-built setup is based on a confocal microscope and employs standard communications-type radiofrequency electronics. Excitation is performed with a cw laser which is amplitude-modulated with an acousto-optic modulator (AOM). Modulation frequencies between 25 and 50 MHz are generated with a computer-controlled direct digital synthesizer (DDS). The fluorescence signal of the sample is demodulated at the fixed frequency of 70 MHz with an I-Q demodulator. Its modulation amplitude and phase shift with respect to the excitation yield information about the fluorescence lifetime(s) in the sample. Single- and bi-exponential fluorescence decays are analysed with a polar-plot technique [1].

[1] G. I. Redford and R. M. Clegg, J. Fluor. **15**, 805 (2005).

CPP 12.3 Mon 16:30 Poster C

Soft x-ray dichroism to explore the molecular orientation using scanning x-ray transmission microspectroscopy (STXM) — •Stephan Wenzel, Andreas Späth, Christian Hub, and Rainer H. Fink — ICMM, Univ. Erlangen, Egerlandstraße 3, 91058 Erlangen, Germany

Scanning transmission soft X-ray microspectroscopy (STXM) has proven excellent spatial resolution (< 20 nm) in combination with spectroscopic information to investigate ultrathin samples. The superior information relies on the photon-energy specific absorption which offers high elemental and chemical contrast. Soft x-ray linear dichroism is established to analyze the molecular orientations in thin film or bulk samples from the angle-dependant absorption. In conventional STXM, the incident angle is fixed by the microscopy geometry. We demonstrate how a rotational device can be used to derive the molecular orientations in organic nano- and microcrystals. We present microspectroscopic studies of TCNQ, NTCDA and NDCI-nanocrystals prepared on commercial Si3N4 membranes. We compare the derived structures from different spectral analysis routines, i.e. stack analysis of images and from line scans. The work is funded by the BMBF under contract 05KS7WE1.

CPP 12.4 Mon 16:30 Poster C

Optical analysis of trap states in amorphous organic semiconductor films — •Harald Graaf[1], Frank Friedriszk[1,2], and Christian von Borczyskowski[1] — [1]Center of nanostructured Materials and Analytics, Chemnitz University of Technology, 09126 Chemnitz, Germany — [2]Institut für Physik, Universität Rostock, 18051 Rostock, Germany

Increasing interest is drawn on thin organic semiconductor films in opto-electronic devices. While for applications like field-effect transistors and photovoltaic cells highly ordered morphologies resulting in higher charge carrier mobilities are requested, for other purposes like organic light emitting diodes amorphous arrangement of the molecules is needed. Here lower mobilities increase the recombination rate leading to a higher photon yield. In such systems trap states can influence dramatically the luminescence in its intensity and spectral regime.

We will show recent results on amorphous films of a perylene dye with a rather high concentration of trap states. These trap states act as sinks for the excitons and leads therefore to a clear shift of the luminescence to the red compared to the monomer emission. Temperature depended and time resolved measurements give a clear hint for the population of the traps from the exciton band. Comparisons with previous electrical measurements lead us to the assumption, that these traps are also dominating the charge carrier mobility within the material.

CPP 12.5 Mon 16:30 Poster C

Enwrapping of tubular J-aggregates using dye-labeled polyelectrolytes — •Omar Al-Khatib[1,2], Helmuth Möhwald[1], Jürgen P. Rabe[2], Christoph Böttcher[3], and Stefan Kirstein[2] — [1]Max-Planck-Insitute of Colloids and Interfaces, Potsdam, Germany — [2]Humboldt University Berlin, Department of Physics, Germany — [3]Freie Universität Berlin, Researchcenter for Electron Microscopy, Germany

In this contribution we demonstrate the coating of tubular J-aggregates with dye-labeled polyelctrolytes. The tubular J-aggregates are formed by an amphiphilic cyanine dye in aqueous solutions [1]. Due to the amphiphilic character of the molecules their aggregates possess a negatively charged surface, which can be utilized for the adsorption of oppositely charged polyelectrolytes. Poly(diallyldimethylammonium chloride) (PDAC)and poly(allylamine hydrochloride) (PAH) labeled with different fluorescent dyes may act as donors or acceptors within a Förster energy transfer (FRET) process.

The enwrapping is verified by cryogenic transmission electron microscopy (cryo-TEM). The FRET is investigated by means of optical absorption and fluorescence spectroscopy. These experiments provide evidence for energy transfer between the aggregate and the dye-labeled polyelectrolyte shell.

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

CPP 12.6 Mon 16:30 Poster C

Spectroscopic and Theoretical Investigations on Pd(II) and Pt(II) Dithiocarbamates — •R. Wenisch[1], D. Forrer[2], S. Gross[2], M. Casarin[2], D. Montagner[2], A. Vittadini[2], M. Helm[1], E. Tondello[2], and S. Gemming[1] — [1]FZ Dresden-Rossendorf, Dresden, Germany — [2]Dept. of Chemistry Univ. Padua, Padua, Italy

In coordination chemistry, the nature and strength of the metal-ligand interaction has attracted much interest. Metal-sulfur complexes, in particular in comparison with their oxygen-based analogues, are intriguing as the sulfur atoms are polarized more easily. The use of specifically tailored sulfur-based ligands allows for tuning the complex functional properties. Among them, electronic properties are very sensitive to changes in the sulfur coordination sphere, suggesting potential uses as molecular switches in optoelectronic devices. Metal dithiocarbamates $[R_2NCS_2]_lM$ have been extensively studied by IR and UV-vis. spectroscopy, ESR and to a limited extent XPS and UPS. Here, we present experimental and theoretical studies investigating the electronic properties of a series of dithiocarbamates of Pd(II) and Pt(II): the pyrrolidine-based one and the 1-pyrrolidinecarbodithioate methyl ester (PyDTM). MX_2(PyDTM) (M = Pt/Pd; X = Cl/Br) were analyzed by XPS and by FT-IR spectroscopy. DFT calculations yielded details on the electronic structure and allowed for unambiguous assignment of the IR spectral features. Ionization energies were evaluated with the asymptotically correct LB94 potential and the two components ZORA.

CPP 12.7 Mon 16:30 Poster C

Coupling of Frenkel excitons, charge transfer excitons and vibrations in linear absorption spectra of polyacene crystals — Ivan Lalov[1,2], •Christoph Warns[2], and Peter Reineker[2] — [1]Faculty of Physics, Sofia University, Sofia 1164, Bulgaria — [2]Institute for Theoretical Physics, Ulm University, 89069 Ulm, Germany

The linear absorption spectra of the crystals of anthracene, tetracene, and pentacene have been calculated in the case of coupling between Frenkel excitons (FEs), charge transfer excitons (CTEs) and intramolecular vibrations. The models and their parametrization for FEs and CTEs in the (a, b) plane of those crystals, first developped by P. Petelenz et al., have been used in the numerical simulations of the linear absorption.

The calculated excitonic and vibronic spectra allow to draw two main conclusions. First, CTEs and their vibronics will manifest themselves in linear absorption of light polarized along the monoclinic axis only (i.e. for tetracene and pentacene along the crystallographic b-axis). Second, the vibronic coupling (FE-phonon and CTEs-phonon) emphasizes and increases the number of the maxima of CTEs manifested in the linear absorption.

CPP 12.8 Mon 16:30 Poster C

Excited states in hole-transporting polymers for phosphorescent OLEDs — •Bianca Höfer[1], Manuel Thesen[2], Silvia Janietz[2], Hartmut Krüger[2], and Anna Köhler[1] — [1]University of Bayreuth, Experimental Physics II, Bayreuth, Germany — [2]Fraunhofer Institute of Applied Polymer Research, Potsdam, Germany

Organic light-emitting diodes (OLEDs) have by now demonstrated efficiencies that enable applications not only for display functions but also for lighting purposes. Current efficient OLEDs are typically fabricated using host-guest-systems. The investigation of excited state formation can help to find ways to suppress efficiency lowering effects like intermolecular excited states. Understanding of the underlying inter- and intra-molecular processes that lead to the formation of excited states can help to optimise host materials. Here we present a comparative spectroscopic study of six hole-transporting materials. These materials consist of a polystyrene backbone with triphenylamine derivatives as pendent side chains. Absorption and photoluminescence measurements as well as time resolved spectroscopy were used to assign emission from singlet, triplet and intermolecular states and determine the transition rates between these states. Furthermore, we discuss the relation between chemical structure and formation of intermolecular states.

CPP 12.9 Mon 16:30 Poster C

Exciton transfer in light-harvesting systems — •Jörg Liebers, Carsten Olbrich, and Ulrich Kleinekathöfer — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

The exciton dynamics in the light-harvesting 2 system (LH2) of purple bacterium are studied with a quantum-classical approach that combines molecular dynamics simulations (MD) with quantum chemistry calculations and quantum dynamical simulations. To obtain the thermal fluctuations of the nuclear positions of the LH2 ring embedded in a membrane, all-atom classical MD simulations were performed. The results of these simulations serve as an input for quantum chemical calculations to determine the energies of the Q_y excited states of the single Bacteriochlorophyll (BChl) molecules. From the results of these calculations we construct a time-dependent Hamiltonian of the LH2 exciton system and the spectral density which describes the interaction of the BChl system and the environment. The exciton dynamics are simulated using two different formalisms. A density matrix approach using the spectral density [1,2] and wave packet dynamics based on the time-dependent Hamiltonian. To compare our approach to experimental results, optical spectra of the LH2 complex are calculated.

[1] U. Kleinekathöfer, J. Chem. Phys. **121**, 2505 (2004).
[2] U. Kleinekathöfer, I. Barvik, P. Herman, I. Kondov and M. Schreiber, J. Phys. Chem. B **107**, 14 094-14 102 (2003).

CPP 12.10 Mon 16:30 Poster C

Transport through a wire with fluctuating site energies — •Bogdan Popescu, Lisa Moevius, and Ulrich Kleinekathoefer — Jacobs University Bremen, Campus Ring 1, 28759, Bremen, Germany

In the present work, the electron transport through a molecule, modeled as a linear chain of tight-binding sites and weakly coupled to external leads, is investigated using a reduced density matrix formalism. A quantum master equation is used in the framework of second-order perturbation theory to describe the dynamics of electrons passing through the molecular wire [1]. The advantage of our method is the accurate treatment of time-dependent effects such as external laser pulses [2]. Our method is applied to compute the electrical current through a molecule, such as DNA, where the site energies and the nearest-neighbor couplings are time dependent because of solvent effects. Moreover, the results are compared to coherent transport calculations on the basis of Landauer theory.

[1] S. Welack, M. Schreiber and U. Kleinekathoefer, The influence of ultra-fast laser pulses on electron transfer in molecular wires studied by a non-Markovian density matrix approach, J. Chem. Phys. 124, 044 712-1-9 (2006).

[2] G.-Q. Li, S. Welack, M. Schreiber and U. Kleinekathoefer, Tailoring current flow patterns through molecular wires using shaped optical pulses, Phys. Rev. B 77, 075 321-1-5 (2008).

CPP 13: Poster: Crystallization and Self Assembly

Time: Monday 16:30–18:00 Location: Poster C

CPP 13.1 Mon 16:30 Poster C

Block copolymer micelles at the solid-liquid interface — •Nicole Voss[1], Marco Walz[1], Stefan Gerth[1], Philipp Gutfreund[2], Max Wolff[3], Hartmut Zabel[2], and Andreas Magerl[1] — [1]Crystallography and Structural Physics, University of Erlangen, Germany — [2]Solid State Physics/EP IV, Ruhr-University Bochum, Germany — [3]Division for Materials Physics, Department of Physics and Material Science, Uppsala University, Sweden

Micellar solutions of block copolymers have rich phase diagrams, which can be controlled by temperature or polymer concentration. Due to the correlation between strucutural properties and macroscopic viscosity the phases can be located using rheometry. A salient result of our investigations is that block copolymer micelles may strongly remember their thermal history. In this regard, a different phase behavior depending on whether heating or cooling the sample can be observed.

Further, these amphiphilic systems are highly sensitive to the properties of a solid boundary. We investigated the solid-liquid interface between aqueous solutions of the copolymer EO(20)-PO(70)-EO(20) and solid walls with different chemical treatments. Using neutron reflectometry we depict the influence of surface energy and temperature on the adsorption behavior of single micelles at solid interfaces. To extract the structural arrangements in concentrated solutions we performed Grazing Incidence Small Angle Neutron Scattering (GISANS) and found a distinct dependance of the near-surface micellar ordering on the surface energy.

CPP 13.2 Mon 16:30 Poster C

Phase behavior of nanorods on quasicrystalline substrates — •Philipp Kählitz and Holger Stark — TU Berlin, Sekr. EW 7-1, Institut für Theoretische Physik Hardenbergstr. 36, D-10623 BERLIN-Charlottenburg

Quasicrystals are structures with long-range positional and orientational order. However, they cannot be periodic since they possess rotational symmetries such as 5- or 10-fold axis that are forbidden for conventional crystals. These structures lead to new and unique features of matter. Therefore, a lot of effort has recently been initiated to grow atomic quasicrystals on quasicrystalline surfaces. To mimic this situation, 2D light-interference patterns have been used to study the phase behavior of micron-sized colloidal particles in a 2D quasicrystalline potential and new ordered phases have been identified [1,2]. This contribution studies the ordering of nanorods, such as organic molecules, in a quasicrystalline substrate potential. By using Monte-Carlo simulations, we have identified varies novel phases. For example, in one phase the centers of mass of the rods order on a hexagonal lattice whereas their orientations display 10-fold symmetry. We demonstrate how these phases are situated in appropriate phase diagrams as a function of the length of the rods , the potential strenght, and the particle density.

[1] Mikhael et al., Nature (London) 454, 501 (2008)

[2] M. Schmiedeberg and H. Stark , PRL 101, 218302 (2008)

CPP 13.3 Mon 16:30 Poster C

Structural Characterization of an amorphous-discotic columnar diblock copolymer, Polystyrene-b-Poly(perylene bisimide acrylate) — •Gaurav Gupta[1], Peter Kohn[1], Michael Sommer[2], Sven Hüttner[2], Thomas Thurn-Albrecht[1], and Mukundan Thelakkat[1] — [1]Institute for Physics, Martin Luther University, Halle, Germany — [2]Applied Functional Polymers, Macromolecular Chemistry I, University of Bayreuth, Bayreuth,Germany

The property of the block copolymers to self assemble into ordered arrays of micro domains have made them an interesting candidate for the fabrication of nanostructured devices. Amongst the various new materials used in organic electronics, discotic materials self assembling into columnar structures are gaining importance as they exhibit one dimensional charge transport and high charge carrier mobility.

We present here the structural characterization of a semiconductor block copolymer, Polystyrene-b-Poly(perylene bisimide acrylate) PS-b-PPBI using temperature dependent XRD, DSC and TEM with an aim to get an insight of the confinement effects on crystallization. The SAXS measurements reveal that the material is microphase separated forming hexagonally packed PPBI cylinders in PS matrix with a spacing of 21nm between them. From TEM results the diameter of this cylindrical micro domain is estimated to be 20nm. The WAXS study shows that the monoclinic crystal structure of PPBI does not change upon confinement in these nanodimensional cylinders. The crystalline structure melts at 1750C resulting in an isotropic liquid.

CPP 13.4 Mon 16:30 Poster C

Substrate induced orientation in thin crystalline polythiophene fims — •Anas Mujtaba, Thomas Henze, Nitin Shigne, and Thomas Thurn-Albrecht — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale)

We studied if and to what extent the crystal orientation of poly (3-hexyl thiophene) thin films can be controlled by substrate effects. Regioregular head-to-tail (HT)-coupled P3HT thin films were crystallized on silicon and HOPG (highly oriented pyrolytic graphite) substrates. Surface morphology and crystal orientation were probed by atomic force microscopy (AFM) and X-ray diffraction (XRD). For both substrates, AFM measurements showed edge-on crystalline lamellae separated by amorphous inter-lamellar zones. The surface topography showed characteristic differences for the two substrates. In some cases for graphite, the crystal orientation reflected the three fold rotational symmetry of the underlying substrate indicating epitaxial effects. XRD measurements revealed different crystal orientation for the two cases. On silicon the crystal a-axis stands perpendicular on the substrate, i.e. the layered structure consisting of separated main and side chains is lying parallel to the substrate, while on graphite the crystal b-axis i.e. the π-π stacking direction is oriented perpendicular to the substrate and consequently the main/side chain layered structure aligned perpendicular to the graphite substrate. The orientation on silicon can be attributed to the wetting effects active in high temperature layered phase, on contrary graphite acts as a nucleating surface inducing oriented epitaxial crystallization.

CPP 13.5 Mon 16:30 Poster C

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, D-06099 Halle (Saale)

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 increases with molecular weight indicates that the semi-crystalline morphology is related to structure of the chains in the amorphous melt before crystallization.

CPP 13.6 Mon 16:30 Poster C

Crystallization kinetics in colloidal model system obtained by small angle light and bragg scattering - a comparison. — •Richard Beyer, Markus Franke, Thomas Palberg, and Hans Joachim Schöpe — Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Germany

We study the crystallization kinetics of spherical colloidal particles with a hard-sphere interaction. The particles are composed of cross-linked polystyrene with a linker/monomer-ratio of 1/10 and are suspended in 2-Ethylnaphtalen with a volume fraction near the melting concentration.

The Bragg light scattering setup allows us to measure a q-range from 4 up to 20 1/um. Further on we have constructed a second machine to measure the scattered light in the small-angle-regime up to 0.7 1/um. Both systems are capable of measuring the full azimuth-angle with a high resolution on the q- and the time-scale giving excellent statistics which allows us to study the crystallization kinetics of our samples.

We present a comparison of the different scattering techniques and of the determined parameters describing the crystallization scenario. The combination of both techniques gives us the possibility to get a comprehensive picture of the crystallization process in colloidal model systems.

CPP 13.7 Mon 16:30 Poster C

Crystallisation in attractive colloidal Hard Spheres — •Richard Beyer, Sara Iacopini, Thomas Palberg, and Hans Joachim Schöpe — Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Germany

We study the crystallization kinetics of a mixture of colloidal "hard-sphere" particles and non-adsorbing polymer, in which the polymer induces a "depletion" attraction between the particles. With increasing amount of added polymer the early stages of the crystallization process are modified significantly and the crystallization process is delayed. We observe obvious deviations from a pure rhcp structure factor and a modification in the time trace and of the absolute values of the nucleation rate density.

CPP 13.8 Mon 16:30 Poster C

Influence of Electric Fields on the Phase Behavior of Concentrated Block Copolymer Solutions — •Heiko G. Schoberth[1,2], Christian W. Pester[1], Kristin Schmidt[3], Kerstin A. Schindler[1,2], and Alexander Böker[1] — [1]Lehrstuhl für Makromolekulare Materialien und Oberflächen and DWI an der RWTH Aachen e.V., RWTH Aachen University, 52056 Aachen, Germany — [2]Lehrstuhl für Physikalische Chemie II, Universität Bayreuth, 95440 Bayreuth, Germany — [3]Materials Research Laboratory, University of California, Santa Barbara, USA

We investigate the influence of the electric field on the phase behavior of diblock copolymers in concentrated solutions using synchrotron small-angle X-ray scattering (synchrotron SAXS). When heating the solutions through the order-disorder transition temperature T_{ODT}, we find a significant decrease in T_{ODT} with increasing electric-field strength. In addition we found a temperature regime in which it is possible to switch between the disordered and phase separated state at constant temperature upon application of a moderate electric field.

Furthermore we can also induce an order-order-transition. We synthesized different block copolymers with compositions close to the predicted phase boundaries. Due to the lower free energy of aligned anisotropic microdomain structures parallel to the electric field, we can induce a transition from the metastable hexagonally perforated lamellae to the lamellae phase under strong electric fields. In addition for an isotropic cubic gyroid phase, which cannot be aligned, a transition to aligned cylinders is found.

CPP 13.9 Mon 16:30 Poster C

Fabrication and Characterization of Two Dimensional Ordered Arrays of Mesoscopic Latex Particles on Solid Surfaces — •Züleyha Yenice and Regine v. Klitzing — Stranski-Laboratorium für Physikalische und Theoretische Chemie - Institut für Chemie TU Berlin, Sekr. TC 9 Strasse des 17. Juni 124 D-10623 Berlin

Textured surfaces of controlled morphology and periodicity are of great significance for many areas of science and technology.

The aim of the present work is to control the distance between particles in a 2D lattice. The deposition of the particles on to the wafer is accruing by spin coating technique [1]. Here the effect of the particle size, different rotational speed, type of solvent and different concentrations of the latex particles in the suspension were examined. For morphological observation an atomic force microscope (AFM) operating in the tapping mode was used.

It was observed that different ionic strengths of the solvent leads to different structures on the surface, the distances between deposited particles decrease with increasing ionic strength. This phenomenon can be explained by the classical DLVO model theory. It was also observed that the viscosity and the evaporation rate of the solvent effects the structure on the surface. However, there is a lack of information about the preparation of high ordered colloidal arrays with the interparticle distance ranging from 10 nm to 100 nm.

[1] P. Jiang, M. J. McFarland. J. Am Chem. Soc. 2004,126, 13778-13786

CPP 13.10 Mon 16:30 Poster C

Photo-initiated Growth of sub-7 nm Silver Nanowires within a Chemically Active Organic Nanotubular Template — •D.M. Eisele[1], H. v.Berlepsch[2], C. Böttcher[2], K.J. Stevenson[3], D.A. Vanden Bout[3], S. Kirstein[1], and J.P. Rabe[1] — [1]Humboldt-Universität zu Berlin — [2]Freie Universität Berlin — [3]Universtiy of Texas at Austin

Silver nanowires are highly promising quasi 1-dimensional nanostructures for a variety of applications in electronics, photonics and catalysis, as well as for sensors. However, it remains a challenge to control their diameters in the interesting range below 10 nm, where their electronic properties begin to deviate substantially from the bulk. Here, it is reported that self-assembled uniform nanotubular J-aggregates of amphiphilic cyanine dye C8S3 [1] can be used as chemically active templates for the photo-initiated fabrication of silver nanowires by reduction of silver salt. The silver ions are reduced by oxidizing the template.[2] Due to the uniformity of the templates, crystalline silver wires have been obtained exhibiting a highly homogeneous diameter of (6.4+/-0.5) nm and lengths exceeding a micron. The nanotubular templates act as structure-directing agents and also as localized chemical reductants for silver ions. They may be functionalized further, e.g. with optoelectronically active polycations, providing access to quasi 1-dimensional organic/inorganic hybrid structures with well defined metallic nanowires as a core. [1] D. M. Eisele et al., Nature Nanotech. 4 (2009) 658; [2] J. L. Lyon et al., J. Phys. Chem. C 112 (2008) 1260.

CPP 14: Poster: Interfaces and Thin Films

Time: Monday 16:30–18:00 Location: Poster C

CPP 14.1 Mon 16:30 Poster C

Random Block Copolymers in the Bulk and at Selective Surfaces — •Birger Steinmüller and Marcus Müller — Institut für Theoretische Physik, Georg-August-Universität Göttingen

The disordered phase of a random block copolymer melt shows structural properties which are of interest for the fabrication of fuel cell membranes. In order to observe their behaviour over larger time and length scales than the ones accessible to atomistic simulations, we employ two different coarse-grained models. The Single-Chain in Mean Field (SCMF) model has soft interactions which allow us to equilibrate our systems very fast, whereas the bead-spring Molecular Dynamics model grants us better access to the real dynamics and the structural properties of the melt.

We quantitatively connect these two different models at large length scales so that we can take advantage of the two models' positive properties. For this, we have found parameter values which result in similar mesoscopic behaviour and then used the SCMF configurations as starting points for MD simulations. Additionally, we look at the behaviour of the melt when in contact with a selectively attractive surface. In our simulations, due to compositional fluctuations, we see a new length scale near the surface, the interphase.

CPP 14.2 Mon 16:30 Poster C

Elastic properties of thin transparent polymer films — •Johannes Wiedersich, Alexander Diethert, Peter Müller-Buschbaum, and Winfried Petry — Physikdepartment E13, TU München, Garching

The method of Brillouin scattering has recently been extended from bulk samples to the application of thin and ultra thin transparent polymer films. The method provides a means to investigate mechanical properties of films with thickness in the nm range in a contactless in-situ manner. Theoretical computations predict a complicated pattern of propagating film and surface guided modes, depending on the thickness and on the mechanical properties of the films, which are spin coated on glass substrates.

We have been able to improve the sensitivity of our Brillouin scattering set-up and extend measurements down to ultra-thin films. The first results on our thinnest films show deviations from the theoretical predictions and indicate that the mechanical modulus deviates from the bulk value for films with thickness on the order of 20 nm.

CPP 14.3 Mon 16:30 Poster C

Polymer chains in confined geometries with long-range correlated disorder. — •Zoryana Usatenko — Universitat Duisburg-Essen, Fachbereich Physik,Duisburg, Germany — Institute for Condensed Matter Physics, Lviv, Ukraine

The influence of long-range correlated disorder of the form $\frac{1}{r^a}$, where $a < d-1$ (and r denotes the distance parallel to the surface) in dilute solution of long-flexible polymer chains in a good solvent on the depletion interaction potential and depletion force between two parallel repulsive walls is studied. The calculations are performed in the framework of renormalization group field theoretical approach up to first order of perturbation theory in a double (ϵ,δ)- expansion ($\epsilon = 4-d$, $\delta = 4-a$) for ϕ^4 $O(n,m)$-vector model in the limit $n,m \to 0$. Besides, the calculations of the monomer density profiles and the density profiles of end points for different regions $L >> R_g$ and $L << R_g$, where L is distance between the walls and R_g - the gyration radius of polymer chain in unrestricted region are performed.

CPP 14.4 Mon 16:30 Poster C

On the Thermodynamics of the 2-dimensional Lamellar Phase of Poly(styrene sulfonate) Adsorbed onto an Oppositely Charged Lipid Monolayer — •Thomas Ortmann, Heiko Ahrens, Jens-Uwe Günther, and Christiante A. Helm — Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Str. 6, D-17489 Greifswald, Germany

Electrostatic and entropic interactions in monolayers of cationic lipids with adsorbed polystyrene sulfonate (PSS) are studied by isotherms, and grazing incidence X-ray diffraction. Dioctadecyldimethylammonium bromide (DODA) is used as lipid, the PSS concentration is 0.01 mM (with respect to the monomer concentration); the PSS chain length is varied. Bragg peaks attributed to flatly adsorbed, aligned PSS chains are observed for PSS both beneath the lipids in the solid (chain separation 2-2.7 nm) and in the fluid phase (chain separation 3-6 nm), the latter only if the PSS contour length exceeds 10 nm. The peak position is independent of the chain length. However the isotherms depend strongly on PSS chain length: the surface pressure of the liquid/condensed phase transition is largest for the shortest PSS used (contour length 5.5 nm) and decreases the longer the polymer gets, a limiting value is reached at 25 nm. The latent heat of the phase transition shows nonmonotic behaviour with an extremum at 8 nm contour length, and levels off at 25 nm. Presumably, for very short PSS chains and large chain separations, the rotational entropy of the electrostatically stretched chains hinders alignment. Even for aligned short chains, the transition enthalpy is affected strongly.

CPP 14.5 Mon 16:30 Poster C

Block Architecture for Neutron Reflectivty Investigation of Internal Interfaces of Polyelectrolyte Multilayers — •Olaf Soltwedel[1], Oxana Ivanova[1], Madlen Müller[1], Ralf Köhler[2], and Christiane A. Helm[1] — [1]Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Str. 6, D-17489 Greifswald, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energien, Glienicker Straße 100, D-14109 Berlin, Germany

Polyelectrolyte multilayer (PEM) are built by sequential adsorption of oppositely charged polyelectrolytes, either poly(styrenesulfonate) - pSS and poly(diallyldimethylammonium) - pDADMAC or poly(allylamine hydrochloride) - pAH solutions. Using neutron reflectivity and a two block PEM architecture, one block consisting of protonated polyelectrolyte bilayers only and one of deuterated bilayers, it is possible to quantify unambiguously the scattering length density and the thickness of the respective blocks. Also, the internal roughness of the interface between the blocks is determined. While the total number of deposited layers is kept constant, the ratio between the protonated and the deuterated block is varied systematically. Different growth zones, i.e. the precursor zone adjacent to the substrate, the core zone and the outer zone next to the air can be distinguished. Depending on the polycation used, not only the internal roughness but also the extension of the zones change within the PEM. Also annealing effects, which appear during preparation of PEM and or after treatment with salt solutions, are investigated with this approach.

CPP 14.6 Mon 16:30 Poster C

In situ measurements of polyelectrolyte multilayers using multiple angle ellipsometry: even-odd effects in layer thickness and refractive index — •Peter Nestler, Stephan Block, and Christiane A. Helm — Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Str. 6, D-17489 Greifswald, Germany

We investigate in situ the growth of polyelectrolyte multilayers (PEMs) by sequential adsorption of poly(allyl amine)hydrochloride (PAH) and poly(styrene sulfonate) (PSS) using multiple angle ellipsometry within a liquid cell. The multilayers are built onto RCA cleaned and poly(ethylen imine) (PEI) coated silicon wafers using polyelectrolyte adsorption solutions, whose temperature is controlled between 22 °C and 55 °C and which additionally contain 1 M NaCl or 1 M KCl. After each adsorption step we determine the PEM thickness and index of refraction with high accuracy by measuring the ellipsometric parameters at several angles of incidence. We observe a PEM thickness which is increased by at least 40% with respect to X-Ray reflectometry measurements performed after drying in air. Furthermore we find, that the increase in PEM thickness after an adsorption step shows an even-odd effect which is attributed to an unequal contribution of both polyelectrolytes to the thickness of one bilayer: at 22 °C PSS amounts to more than 60% to the average bilayer thickness, whereas at 55 °C this value reduces to 35%. A similar even-odd effect is observed in the refractive index of the PEM and allows an estimation of the refractive index of a single PSS or PAH layer within one bilayer.

CPP 14.7 Mon 16:30 Poster C

Layer-by-layer fabrication of hierarchical structures in sol-gel templated thin titania films — •Jan Perlich[1,2], Mine Memesa[3], Alexander Diethert[1], Ezzeldin Metwalli[1], Weinan Wang[1], Stephan V. Roth[2], Andreas Timmann[2], Jochen S. Gutmann[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department LS E13, Garching — [2]HASYLAB at DESY, Hamburg — [3]Max-Planck-Institute for Polymer Research, Mainz

Nanostructured titania thin films have gained great popularity in a variety of applications such as coatings, photocatalysis, gas sensing, and photovoltaics. For most of these applications a defined morphology of the titania nanostructures is crucial for the functionality and significantly influences the performance. The morphology determines the volume-to-surface ratio and hence the surface available for interfacial reactions. In order to increase the surface area the fabrication of titania nanostructures with hierarchical order of different structural levels is investigated. The nanostructures are prepared with a diblock-copolymer assisted sol-gel process. By iterative spin-coating of the solution onto silicon substrates a thin polymer-nanocomposite film is deposited and transformed to purely anatase titania nanostructures via calcination. This procedure is repeated three times on top of the substrate. The approach is monitored with grazing incidence small angle X-ray scattering (GISAXS) performed at the synchrotron beamline BW4 of DESY HASYLAB after each fabrication step. With scanning electron microscopy the final hierarchical structure is imaged. From the characterization different structural levels are clearly identified.

CPP 14.8 Mon 16:30 Poster C

Ordering of amphiphilic particles at a hard wall — •Gerald Rosenthal and Sabine H. L. Klapp — Institut für Theoretische Physik, Fak. II, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin

We present a numerical calculation of amphiphilic molecules at a hard wall using density functional theory. We focus on the competition between surface field and interaction-induced ordering phenomena. Amphiphilic molecules (e.g. surfactants, Janus-particles) are composed of hydrophilic and hydrophobic segments. We use an effective coarse-grained model, which describes the "surfactants" or Janus-particles as hard spheres with a hydrophilic and a hydrophobic side. This anisotropy is realized by a vector as an internal degree of freedom. The coarse-grained model goes back to Tarazona *et al.* [1]. In our density functional approach we use the White-Bear fundamental measure theory [2] for the hard sphere part and a mean-field approximation for the anisotropic part of the interaction.

[1] A. M. Somoza, E. Chácon, L. Mederos and P. Tarazona, J. Phys.: Condens. Matter **Vol. 7**, 5753 (1995).

[2] H. Hansen-Goos and R. Roth, J. Phys.: Condens. Matter **Vol. 18**, 8413 (2006).

CPP 14.9 Mon 16:30 Poster C

Modification of the electrical conductivity in conjugated polymer films — •Andreas Nathan[1], Matthias A. Ruderer[1], Robert Meier[1], Hyeokmin Choe[1], Robert Cubitt[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department LS E13, James-Franck-Str. 1, 85747 Garching, Germany — [2]Institut Laue-Langevin, 6 rue Jules Horowitz, 38000 Grenoble, France

Conjugated polymers in thin films are of great interest for various applications such as organic photovoltaics, organic light emitting diodes and organic field effect transistors. Therefore, the selective modification and control of their electrical conductivity has special importance. Doping of conjugated polymers in particular allows for the adjusting of the conductivity. In polyacetylene the conductivity is increased over a remarkably large range from an insulating to a metallic behaviour.

In this work we prepare thin films of polyacethylene derivatives through solution based processes and test different doping methods. The film thickness is determined with x-ray reflectivity measurements. The electrical conductivity is measured with respect to film thickness and doping. UV/Vis measurements complete our investigations.

CPP 14.10 Mon 16:30 Poster C

Electrical properties of a charge-transfer interlayer modified organic heterojunction — •Shuwen Yu[1], Ingo Salzmann[1], Antje Vollmer[2], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Institut f. Physik, Brook-Taylor-Str. 6, 12489 Berlin — [2]HZB-BESSY, Albert-Einstein-Str. 15, 12489 Berlin

We investigated the effect of a thin interlayer (ca. monolayer) of tetrafluoro-tetracyanoquinodimethane (F4-TCNQ) between prototypical hole and electron transport layers (HTL and ETL) on interface energetics and current transport. As HTL we used 4,4',4"-tris(N,N-diphenyl-amino)triphenylamine (TDATA) and tris (8-hydroxyquinoline)aluminium (Alq3) as ETL, which are commonly employed in organic light emitting diodes. The hole injection barrier into TDATA is 0.5 eV, as measured by photoemission spectroscopy. Deposition of an F4-TCNQ interlayer on top of TDATA does not further change the energy level position. However, after applying the F4-TCNQ interlayer the energy levels of Alq3 deposited on top of TDATA are 0.15 eV closer to the Fermi-level than without the interlayer. Diodes fabricated without interlayer had a 0.6 V higher onset-voltage one order of magnitude lower current density than those with F4-TCNQ. These observations can be rationalized by an increased (non-radiative) electron-hole recombination rate at the modified organic heterojunction and a changed internal electric field distribution.

CPP 14.11 Mon 16:30 Poster C

Active microrheology of (Gibbs) monolayers — •Uli Langer and Thomas Fischer — Universität Bayreuth, Bayreuth, Germany

We describe the setup of a nano-needle rheometer, in order to measure the surface viscosity of monolayers. The reorientation of nickel nanorods in an external magnetic field is analysed in order to obtain the surface shear viscosity.

CPP 14.12 Mon 16:30 Poster C

Interfacial effects on single dye diffusion in ultrathin liquid films — •Daniela Täuber, Frank Gerlach, Sebastian Schubert, and Christian von Borczyskowski — TU-Chemnitz, Institut für Physik, 09107 Chemnitz, and FOR 877

Liquids show layering at solid-liquid interfaces [1], which leads to dynamic heterogeneity in diffusion. Recent observations show additional influence of static heterogeneities of the interface on diffusion.

Here we used Rhodamines to trace the diffusion in ultrathin liquid (TEHOS) films on Si wafers with thermally grown oxide via optical single molecule tracking. Long term observations on thinning films reveal that there is no change in diffusion down to three molecular diameters from the substrate [2]. On the other hand modification of the silanol density on the substrate influenced the fraction of near surface diffusion. Enhancement of diffusion was correlated with the silanol cluster size (ca 0.5 microns) on the heterogeneous substrate.

[1] C.-J. Yu et al: , Phys. Rev. Lett. 82 (1999) 2326-29

[2] D. Täuber, C. von Borczyskowski et al: Diff. Fund. J. 12 (2009) accepted

CPP 14.13 Mon 16:30 Poster C

Kinetics studies of lamellar poly(styrene-b-butadiene) diblock copolymer thin films during heat treatment — •Alessandro Sepe[1], Zhenyu Di[1], Tilo Hoppe[1], David Magerl[1], Jan Perlich[4], Dorthe Posselt[2], Detlef-M. Smilgies[3], and Christine M. Papadakis[1] — [1]TU Munchen, Physikdepartment E13, Garching, Germany — [2]Institute for Science, Systems and Models, Roskilde University, Denmark — [3]Cornell High-Energy Synchrotron Source (CHESS), Ithaca, U.S.A. — [4]HASYLAB at DESY, Hamburg

Nanostructured block copolymer thin films find a number of applications, especially as templates for anorganic materials, which may be used as optical elements or data storage devices. Thermal treatment has been applied to improve the orientation and the long-range order of the mesostructure.

We have studied thin films of lamellar poly(styrene-b-butadiene) (P(S-b-B)) diblock copolymers to elucidate the mechanisms of structural changes induced by thermal treatment and their kinetics. The lamellae initially have the perpendicular lamellar orientation. In-situ, real-time grazing-incidence small-angle X-ray scattering, as well as ex-situ atomic force microscopy and X-ray reflectometry were used. We found that the processes during thermal annealing strongly depend on the treatment temperature: Below the glass-transition temperature of the PS block, the perpendicular orientation is unchanged, whereas above, a more random lamellar orientation is observed and the film surface is flattened.

CPP 14.14 Mon 16:30 Poster C

Very slow breakout crystallization in cylinder-forming diblock copolymer thin films — •Christine M. Papadakis[1], Charles Darko[1], Zhenyu Di[1], Kordelia Troll[1], Ezz Metwalli[1], Andreas Timmann[2], Günter Reiter[3], and Stephan Förster[4] — [1]TU München, Physikdepartment E13, Garching — [2]HASYLAB at DESY, Hamburg — [3]Albert-Ludwigs-Universität Freiburg, Fakultät für Physik und Mathematik — [4]Universität Hamburg, Department Chemie

In thin polymer films, crystallization often leads to fascinating surface structures. We have investigated the long-term behavior of the crystallization in thin films of cylinder-forming poly(isoprene-*b*-

ethyleneoxide), PI-*b*-PEO. Using optical microscopy, AFM, X-ray reflectometry and grazing-incidence wide- and small-angle X-ray scattering, we have observed very slow breakout crystallization of the PEO. The crystallization of the film was complete only after 150 days. The original hexagonal morphology was destroyed by crystalline lamellae lying in the film plane. The PEO chain stems were perpendicular to the film plane. We attribute this slow breakout to the shortness of the PEO blocks which change from being amorphous in the confinement of the cylinders to twice-folded in the lamellae.

CPP 14.15 Mon 16:30 Poster C

Structural rearrangements in a lamellar diblock copolymer thin film during treatment with saturated solvent vapor — Zhenyu Di[1], Dorthe Posselt[2], Detlef-M. Smilgies[3], and •Christine M. Papadakis[1] — [1]TU München, Physikdepartment E13, Garching — [2]IMFUFA, Roskilde University, Denmark — [3]CHESS, Cornell University, USA

The processes during vapor treatment of block copolymer thin films, which is often used for equilibrating film structures, are complex. Solvent not only swells the polymers, but also increases the chain mobility and reduces the interfacial tension between the blocks [1].

We have investigated the structural changes in thin films of lamellar poly(styrene-b-butadiene) diblock copolymers during treatment with saturated cyclohexane vapor, a solvent slightly selective for polybutadiene. Using real-time, in-situ grazing-incidence small-angle X-ray scattering (GISAXS) [2], the swelling and the rearrangement of the lamellae were investigated with a time resolution of a few seconds. After a few minutes in vapor, a transient state with a more well-defined and more long-range ordered lamellar orientation was encountered. Additional parallel lamellae formed because of the increased degree of coiling of the polymers in the swollen state. Eventually, the film became disordered.

[1] C. M. Papadakis et al., Langmuir 24, 13815 (2008). [2] D.-M. Smilgies et al, Mater. Res. Soc. Symp. Proc. 1147, OO01-01 (2009) [3] Z. Di, et al., Macromolecules, accepted.

CPP 14.16 Mon 16:30 Poster C

Density and Viscosity at the polymer-solid interface — •Eicke Tilo Hoppe, David Magerl, and Christine M. Papadakis — TU München, Physikdepartment E13, Garching

Close to the interface between a polymer film and a solid, the polymer properties may deviate from the bulk. This change in physical behavior is of importance for the adhesion of polymer coatings to solids, e.g. in medical implants or in paints.

The aim of the project is the investigation of the influence of the polymer-solid interaction on the physical properties of the polymers near the interface. The focus lies in the correlation between the change of density and viscosity of the polymer near the interface.

Polybutadiene melts on dry thermally oxidized silicon are studied as a model system. The changes in density and viscosity are investigated by neutron reflectometry and fluorescence correlation spectroscopy. To tune the interface interactions between substrate and polymer melt, the substrate surface is modified by different silanizations.

CPP 14.17 Mon 16:30 Poster C

How do co- and counter ions affect 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.[1,2] 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 freestanding 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)[3]. This method has been successfully used to proof 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, M. Armélin, G.H. Findenegg, R. v. Klitzing, Langmuir 2005, 21, 4790 [2] C.L. Henry, C.N. Dalton, L.Scruton, V.S.J. Craig, J. Phys. Chem. C 2007, 111, 1015 [3] R. v. Klitzing, Adv. Coll. Interf. Sci. 2005, 114/115, 253 [4] K. Hänni-Ciunel, N. Schelero, R. v. Klitzing, Faraday Discussion, 2009, 141, 41

CPP 14.18 Mon 16:30 Poster C

Molecularly imprinted PPy for the voltage-dependent uptake and release of L-glutamate in neutral pH — •Kathrin Fuchs, Elizabeth von Hauff, and Jürgen Parisi — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, Carl-von-Ossietzky Str. 9-11, 26129 Oldenburg, Germany

For medical or biological applications, a device, which can control the concentration of a specific biomolecule in solution, is of great interest. Therefore, polypyrrole (PPy) is analysed with respect to the voltage-dependent uptake and release of L-glutamate, an important neural transmitter in the human nervous system. Additionally the effect of glutamate diffusion out of the film is investigated.

The PPy is electrochemically deposited on Au-coated electrodes utilizing an aqueous solution containing the monomer pyrrole and sodium L-glutamate. For some examinations, the PPy was electrochemically overoxidized using a phosphate buffer solution and thereby creating glutamate selective cavities. Such overoxidized PPy films have been described as having selective properties regarding the L-conformation of glutamate at low pH [1]. In this study, the uptake and release of glutamate resulting from a voltage sweep and having a mass change of the polymer film in neutral pH solution as a consequnece is measured using an electrochemical quartz crystal microbalance (EQCM), while the diffusion of glutamate out of the polymer film is determined using UV/Vis-spectroscopy.

[1] B. Deore, Z. Chen, and T. Nagaoka, Analytical Sciences, 15, 827, 1999

CPP 14.19 Mon 16:30 Poster C

Temperature-dependent structure transitions in thin smectic liquid crystalline films — •Benjamin Schulz, Christian Bahr, and Stephan Herminghaus — MPI for Dynamics and Self-Organization, Bunsenstraße 10, 37073 Göttingen

Thin films of smectic liquid crystals are known to show the formation of self-organized structures if they are subjected to antagonistic boundary conditions [1]. Such structure formations are promising systems as templates for the lithography of photonic crystals [2]. For this reason, a deeper understanding of the conditions that evoke different types of such structures is necessary for further applications of liquid crystal films.

We study films of about 300 nm in thickness of the liquid crystal 8CB near its transition between the smectic-A and the nematic phase using AFM and optical microscopy/polarized light microscopy. Below the actual phase transition temperature, we find structural changes in both the internal structure of the film and the surface topography. Depending on the film thickness, we can identify up to three different structures in the smectic phase. The liquid nature of our system should allow for a straightforward minimization of the free energy. However, near the second-order transition to the nematic state this seems to be a delicate process as we observe different structures. This behaviour could result from major changes of the elastic properties of the film in the vicinity of the transition.

CPP 14.20 Mon 16:30 Poster C

Alignment Mechanism of SVT Polymer Thin Films and its 3-Dimensional Characterization: A Combined QIS-SFM Imaging Study — •Clemens Liedel[1], Markus Hund[2], Violetta Olszowka[2], and Alexander Böker[1] — [1]Lehrstuhl für Makromolekulare Materialien und Oberflächen und DWI an der RWTH Aachen e.V., RWTH Aachen University, D-52056 Aachen, Germany — [2]Lehrstuhl für Physikalische Chemie II, Universität Bayreuth, D-95440 Bayreuth, Germany

We observe the direct current electric field induced alignment in thin polymer films with cylindrical morphology basing on a hexagonal superstructure.

So far, little is known about the exact mechanism leading to microdomain orientation of polymer systems in the border region between cylinders and perforated lamellae. Here, we describe quasi *in-situ* scanning force microscopy (QIS-SFM) measurements on thin films of a linear polystyrene-*b*-poly(2-vinylpyridine)-*b*-poly(*tert*-butyl methacrylate) triblock copolymer under an electric field. The alignment process is followed using a new SFM design which enables solvent vapor and electric field treatment after each scanning cycle.

The orientation mechanism is studied and compared to the mechanisms in lamellar block copolymer morphologies. Rotation and nucleation-and-growth mechanisms and defect movement, basing on a hexagonal superstructure, are observed leading to a long-range ordered morphology of aligned core-shell cylinders.

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CPP 14.21 Mon 16:30 Poster C

Self Stratification in polymer blend films during spin-coating — •Cheng Huang[1], Jörg Pfeifer[1], Stefan Walheim[1], and Thomas Schimmel[1,2] — [1]Institute of Nanotechnology (INT), Northern Campus, Karlsruhe Institute of Technology (KIT) — [2]Institute of Applied Physics, Southern Campus, Karlsruhe Institute of Technology (KIT)

The phase separation process of PS/PMMA blend during spincoating from a Methy-Ethyl-Ketone (MEK) solution is studied. The polymer blend dissolved in this solution forms a purely lateral structure on a hydrophilic substrate with PS cylinders in PMMA matrix. Our results of time-resolved in situ reflectometry, post cast ellipsometry and SEM(scanning electron microscope) cross-sectional analysis point in the direction of a transient triplelayer formation during the spincoating process which then transforms via an instability into the final lateral morphology. A purely horizontally layered situation in the dry state can also be tuned by process parameters. 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 for further applications.

CPP 14.22 Mon 16:30 Poster C

High Aspect Ratio Constructive Nanolithography with a Photo-Dimerizable Molecule — Matthias Barczewski[1], •Alexander Förste[1], Stefan Walheim[1], Tobias Heiler[1], Alfred Blaszczyk[1,2], Marcel Mayor[1,3], and Thomas Schimmel[1,4] — [1]Institute of Nanotechnology (INT), Northern Campus, Karlsruhe Institute of Technology (KIT) — [2]Department of Commodity Science, Poznan University of Economics, Poland — [3]Department of Chemistry, University of Basel, Switzerland — [4]Institute of Applied Physics, Southern Campus, Karlsruhe Institute of Technology (KIT)

A major challenge in constructive nanolithography is the preservation of the lateral resolution of a monolayer-thick template pattern while amplifying it to a structure with a thickness above 10 nm. Our approach of photoinduced, constructive, reversible nanolithography, is based on nanografting within a coumarin-derivative thiol (CDT) solution using the tip of an atomic force microscope (AFM). By photodimerization and the formation of disulfide bonds, the CDT polymerizes in a single-step process. We demonstrate the highest lateral resolution in constructive nanolithography at thicknesses above 10 nm (40nm lateral resolution at 12 nm thickness, aspect ratio: 0.3).

CPP 14.23 Mon 16:30 Poster C

Self-Alignment of Block Copolymers on Chemically Patterned Substrates — •Tobias Heiler[1], Roland Gröger[1], Stefan Walheim[1], and Thomas Schimmel[1,2] — [1]Institute of Nanotechnology (INT), Northern Campus, Karlsruhe Institute of Technology (KIT) — [2]Institute of Applied Physics, Southern Campus, Karlsruhe Institute of Technology (KIT)

Chemical patterns were made by nanoshaving polymer brush layers on silicon oxide. The contrast in polarity between brush surface and exposed silicon oxide was used to control the phase morphology of an amphiphilic block copolymer film. The two components of the block copolymer, as well as the surface of the chemically patterned substrate possess a high contrast in polarity, so that a defect tolerant pattern replication in the polymer film is observed after a short (vapor-)annealing process. Polybutadiene-based block copolymers and polystyrene brushes were used.

CPP 14.24 Mon 16:30 Poster C

Influence of connectivity on the entropic stiffness of tethered membranes — •Marco Werner[1,2] and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Germany — [2]Technische Universität Dresden - Institute for Theoretical Physics

We investigate the static and dynamical properties of tethered structures like membranes and fractal polymer objects using the Bond-Fluctuation-Model in three-dimensional space. Tethered structures can be characterized by the spectral dimension depending on their connectivity. For two-dimensional polymers (perfect membranes) we confirm the picture of an entropic stiffness induced locally by excluded volume interaction, which in turn causes a flat state on larger scales [Y.Kantor and K.Kremer, *Phys. Rev. E* 48(4), 2490, (1993)]. On the other hand we found fractal structures e.g. Sierpinski gaskets to be crumpled and their fractal dimension to agree with mean-field arguments [M.E.Cates, *Phys. Rev. Lett.* 53(9), 926, (1984)], whereas Sierpinski carpets are asymptotically flat like perfect membranes. Indeed we found mean field arguments to be self consistent for Sierpinski gaskets but not for Sierpinski carpets. Thus the lower critical dimension for tethered membranes might be below 2 as indicated by an ϵ-expansion [J.A.Aronovitz and T.C.Lubensky, *Phys. Rev. Lett.* 60(25), 2634, (1988)].

CPP 14.25 Mon 16:30 Poster C

Effect of chain architecture on microdomain orientation in thin films of block copolymer supramolecular assemblies — •Bhanu Nandan and Manfred Stamm — Leibniz-Institut für Polymerforschung Dresden, Hohe Strasse 6, 01069 Dresden

The phase behaviour of supramolecular assemblies (SMA) formed by poly(4-vinylpyridine)-b-polystyrene-b-poly(4-vinylpyridine) (P4VP-b-PS-b-P4VP) triblock copolymer with 2-(4'-hydroxybenzeneazo)benzoic acid (HABA) was investigated with respect to the molar ratio (X) between HABA and 4VP monomer unit. The results were compared with SMAs formed by a PS-b-P4VP diblock copolymer of similar composition as the triblock but half the molecular weight to ascertain the effect of chain architecture on microphase separation. In bulk, both the di- and triblock SMAs showed composition dependent morphological transitions which could be tuned by HABA/4VP molar ratio. In thin films also, both the di- and triblock SMAs showed more or less similar morphological transitions depending on X. Interestingly, the domain orientation of the cylindrical or lamellar microdomains in the SMAs was influenced by the chain architecture of the block copolymer. After chloroform annealing whereas the diblock SMAs showed in-plane orientation of the domains, triblock SMAs showed perpendicular domain orientation. The perpendicular orientation of the microdomains in triblock was favored since it allowed the mid PS blocks to acquire normal distribution of loop and bridged conformations. *This research was supported by the priority program of DFG (SPP1165, Project No. STA324/31).

CPP 14.26 Mon 16:30 Poster C

High Density Magnetic Nanorods via Electrodeposition in Block Copolymer Thin Film Templates — •Marcus Böhme, Bhanu Nandan, and Manfred Stamm — Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden

Recently, we presented a Nanotemplate based on the Supramolecular Assembly of poly-(styrene-b-4-vinylpyridine) with 2-(4'-hydroxybenzeneazo)benzoic acid[1]. One possible application of these templates is the creation of high density magnetic rod arrays to overcome the superparamagnetic limit in magnetic storage devices. Requirements for possible application are long range order and homogeneous filling of the individual pores.

Here, we present our results on increasing the long range order via solvent vapor treatment and filling the template pores with magnetic materials, e.g. cobalt, via electrochemistry. [1]A. Sidorenko, I. Tokarev, S. Minko, M. Stamm; JACS 125, 12211-12216, (2003)

CPP 14.27 Mon 16:30 Poster C

Supramolecular assembly of poly(styrene)-b-poly(4-vinylpyridine) and 1-pyrenebutyric acid in thin film and their use for nanofabrication — •Biplab Kumar Kuila and Manfred Stamm — Department of Nanostructured Materials, Leibniz Institute of Polymer Research Dresden, Hohe Str. 6, D-01069 Dresden, Germany.

Block copolymer(BCP)based supramolecules are prepared by attaching small additive molecules in to the side chains of one of the BCP blocks1. BCP-based supramolecules also microphase separate similar to block copolymer into arrays of microdomains, tens of nanometers in size. Here, we have studied the supramolecular assembly of 1-pyrenebutyric acid(PBA)with PS-b-P4VP [Poly(styrene-block-(4-vinyl pyridine). The supramolecular assembly of PS-b-P4VP with PBA resulted the switching of block copolymer morphology from cylinder to lamella in thin film due to compositional change.PBA will make supramolecules with the P4VP block due to strong hydrogen bonding between the carboxylic group of 1-pyrenebutyric acid and pyridine ring of P4VP. After fabricating the thin film from the supramolecules, the minor component PBA can be easily removed by dissolving the thin film in ethanol to transform the block copolymer thin film into nanotemplate or membrane for practical application. We have also observed that these nanotemplates can be used for the fabrication of arrays of nanowire of different functional material like metal or semiconductor. Reference: 1.Sidorenko, A.; Tokarev, I.; Minko, S.; Stamm, M. J. Am. Chem. Soc. 2003, 125, 12211.

CPP 14.28 Mon 16:30 Poster C

Functionalization of Nanostructures via Covalent Binding of Molecules — •Thomas Baumgärtel, Harald Graaf, and Christian von Borczyskowski — Center of Nanostructured Materials and Analytics, Institut für Physik, TU Chemnitz, 09107 Chemnitz, Germany

Anchoring functional molecules or nanoparticles to silicon substrates is a field of increasing interest as it can be employed to create tuneable and well-defined surfaces with various properties and functions. The formation of e.g. self-assembled monolayers of molecules on silicon or silicon oxide surfaces is a process which is basically understood and can be carried out using different chemical routes. However, if such a chemical surface functionalization is carried out in a multi-stage procedure on confined geometries, e.g. nanostructures, there are many problems to be dealt with. Amongst others it is desirable to anchor the molecules via covalent bonds which are much more stable compared to physisorption or electrostatic binding. We will report on the creation and functionalization of nanostructures on SAM-terminated silicon surfaces using different types of molecules and chemical routes. The nanostructures are produced by AFM-induced local anodic oxidation of the silicon. The generated structures are characterized by AFM and Kelvin Probe Force Microscopy. Nanostructures functionalized with optically active molecules or nanocrystals are additionally investigated using spectrally and temporally resolved confocal microscopy.

CPP 14.29 Mon 16:30 Poster C

Mapping sub-surface features in heterogenous polymers — •Eike-Christian Spitzner, Christian Riesch, and Robert Magerle — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

We study tip-sample interaction during scanning force microscopy (SFM) in intermittent contact mode on thin films of polystyrene and polystyrene-*block*-polybutadiene block copolymer swollen in chloroform vapor as well as semicrystalline polypropylene. We measure pointwise amplitude and phase as function of tip-sample distance (apd curves) and determine conservative and dissipative contributions to the interaction process. In addition we obtain the amount of tip indentation into the polymer film. As a result, maps of apd curves provide depth resolved information about structures at and beneath the surface. The accessible depth is limited by the maximal tip indentation that can reach values up to 30 nm for very soft materials.

CPP 15: Poster: Nuclear Magnetic Resonance - Frontiers and Applications

Time: Monday 16:30–18:00 Location: Poster C

CPP 15.1 Mon 16:30 Poster C

A novel approach to high-pressure nuclear magnetic resonance in diamond anvil cells — •Thomas Meissner[1], Swee Kuan Goh[2], Damian Rybicki[1], Benno Meier[1], Grant Williams[3], and Jürgen Haase[1] — [1]Faculty of Physics and Earth Science, University of Leipzig, Germany — [2]Cavendish Laboratory, University of Cambridge, United Kingdom — [3]Industrial Research, Lower Hutt, New Zealand

In addition to variation of temperature and application of external magnetic fields the electronic properties of many materials may be influenced by application of pressure. The highest pressures can be achieved in diamond anvil cells (DAC) but limited sample size and anvil cell geometry hampered their application in nuclear magnetic resonance (NMR) experiments due to a weak signal-to-noise. Recently we succeeded in improving the sensitivity of NMR measurements in DACs significantly by placing the radio-frequency coil containing the sample in the high-pressure region. Here we report on first high-sensitivity measurements at pressures up to 70 kbar.

CPP 15.2 Mon 16:30 Poster C

EPR and NMR of Multiferroic Eu$_x$Ba$_{1-x}$TiO$_3$ — •Nataliya Georgieva[1], Andreas Pöppl[1], Rolf Böttcher[1], Marko Bertmer[1], Jürgen Haase[1], and Alex Sushkov[2] — [1]Faculty of Physics and Earth Sciences, University of Leipzig, Germany — [2]Physics Department, Yale University, New Haven, Connecticut

We are investigating multiferroic Eu$_x$Ba$_{1-x}$TiO$_3$ with different Eu^{2+} concentrations (x = 1, 0.75, 0.5, 0.25) using Electron Paramagnetic Resonance (EPR) and Nuclear Magnetic Resonance (NMR) spectroscopy. The ceramic samples exhibit different magnetic and electric properties, depending on their Eu^{2+} concentration. The X- and Q-band EPR spectra show almost isotropic exchange-coupled Eu^{2+} signals. Temperature dependent line broadening effects are observed and differ for various Eu^{2+} concentrations. ^{137}Ba NMR spectra were recorded using frequency stepped Hahn Echo experiments and preliminary ^{47}Ti/^{49}Ti NMR measurements were recorded. The line width of the central ^{137}Ba nuclear quadrupole transition shows a striking dependence on the Eu^{2+} concentration.

CPP 15.3 Mon 16:30 Poster C

Spatial inhomogeneities in optimally doped and underdoped high-temperature superconducting single crystals of $HgBa_2CuO_{4+d}$, a ^{63}Cu and ^{199}Hg NMR study — •Damian Rybicki[1,2], Juergen Haase[1], Marc Lux[1], Martin Greven[3,4], Guichuan Yu[5], and Yuan Li[5] — [1]Faculty of Physics and Earth Sciences, Leipzig University, Linnéstraße 5, 04103 Leipzig, Germany — [2]Department of Solid State Physics, Faculty of Physics and Applied Computer Sciences, AGH-University of Science and Technology, Al. Mickiewicza 30, 30-059 Krakow, Poland — [3]School of Physics and Astronomy, University of Minnesota, 116 Church Street S. E. Minneapolis, MN, 55455, USA — [4]Stanford Synchrotron Radiation Laboratory, Stanford, CA 94309, USA — [5]Department of Physics, Stanford University, Stanford, CA 94305, USA

Nuclear magnetic resonance is a very important tool to study high-temperature superconducting cuprates (HTSCs). We present results of ^{63}Cu and ^{199}Hg NMR of $HgBa_2CuO_{4+d}$ single crystals with critical temperatures, T_c=97 K and T_c=74 K (optimally doped and underdoped, respectively). $HgBa_2CuO_{4+d}$ due to its very simple structure and only one Cu lattice site is a model compound for understanding the properties of HTSCs. Measurements of the central and satellite transition lines have been carried out as a function of temperature (20-300 K) and orientation of the external magnetic field, B_0 with respect to crystal axes. From the temperature dependence of the spin shifts, line widths and quadrupole splitting we find a very large spatial variation of the hole density even in these high quality single crystals.

CPP 15.4 Mon 16:30 Poster C

Modeling NMR and EPR Parameters in the Metal-Organic Framework Cu3(BTC)2 — •Nina Vankova and Thomas Heine — Jacobs University Bremen, School of Engineering and Science, Bremen, Germany

In the last decade metal-organic frameworks (MOF) have been the subject of intensive research activity due to their tunable porous structure promoting interesting properties and applications. A very powerful tool for characterization of the complex chemical and electronic structure of these nanoporous materials is magnetic resonance spectroscopy. The interpretative and analytical power of the applied NMR and EPR experimental techniques can be significantly enhanced by supplying a reliable theoretical treatment of the underlying spectroscopic parameters.

We report on the application of density functional theory (DFT) for computing the magnetic resonance properties of Cu3(BTC)2(H2O)3 (BTC = benzene 1,3,5-tricarboxylate). The ADF 2008 code with Slater basis sets incorporating relativistic corrections has been used for geometry optimization of the MOF building block. We have performed gas phase calculations modeling both the ground singlet and the excited triple state of the Cu(II) ions from the paddle-wheel unit. The nuclear shielding tensors of C and H forming the BTC linkers, as well as the ESR g- and A-tensors of the Cu(II) ions in the paddle-wheel have been calculated and compared to experimental results from the literature.

CPP 15.5 Mon 16:30 Poster C

NMR in pulsed magnetic fields — •Benno Meier[1], Jürgen Haase[1], Frederik Wolff-Fabris[2], Thomas Herrmannsdörfer[2], and Joachim Wosnitza[2] — [1]University of Leipzig, Institute for

Experimental Physics II, Magnetic Resonance of Complex Quantum Solids — [2]Hochfeld-Magnetlabor Dresden (HLD), Forschungszentrum Dresden-Rossendorf (FZD)

The first observation of NMR in the pulsed high magnetic field at the Hochfeldmagnetlabor Dresden (HLD), Forschungszentrum Dresden-Rossendorf (FZD) is reported. The new spectrometer that operates at up to 3.0 GHz is described, as well as its implementation in the pulsed field facility. Free induction decays and spin echo experiments on ^{1}H and ^{63,65}Cu in various magnets will be described and discussed in terms of sensitivity and resolution.

CPP 15.6 Mon 16:30 Poster C

17O and 63Cu NMR of electron-doped High-Temperature Superconductor Pr1.85Ce0.15CuO4 — •Michael Jurkutat[1], Grant Williams[2], Damian Rybicki[1], and Jürgen Haase[1] — [1]Universität Leipzig, Fakultät für Physik und Geowissenschaften, Postfach 100920, 04009 Leipzig, Germany — [2]The MacDiarmid Institute, Industrial Research, P.O.Box 31310, Lower Hutt 5040, New Zealand

We present results of a nuclear magnetic resonance (NMR) study of c-axis aligned powder samples of the electron-doped high temperature superconducting cuprate Pr1.85Ce0.15CuO4. In particular the effect of partial Ni substitution for Cu on 63Cu NMR is investigated as a function of temperature, crystal orientation and Ni substitution. We find Ni-induced broadening of the spectra and temperature-dependent effects on spin-lattice relaxation indicating spin density oscillations about the Ni site. Furthermore we analyse the temperature and field dependence of 17O NMR spectra showing unexpected resemblances to hole-doped systems.

CPP 15.7 Mon 16:30 Poster C

Chain Dynamics of Polymers Confined to Ordered Nanoporous Alumina Membranes — Cornelius Franz[1], •Salim Ok[2], Fabián Vaca Chávez[1], Martin Steinhart[2,3], and Kay Saalwächter[1] — [1]Institut für Physik, Betty-Heimann-Str.7, 06120 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — [3]Institut für Chemie, Barbarastr. 7, Universität Osnabrück, 49069 Osnabrück, Germany

Ordered anodic aluminum oxide (AAO) membranes with cylindrical 20-400nm pores are ideal inorganic model components that allow studying polymeric interphases and confinement effects in nanocomposites. Advanced NMR techniques enable characterization of polymer chain dynamics in detail. We report the study of polybutadiene (PB) melts infiltrated into AAO by means of transverse relaxometry (T2) as a qualitative indicator for changes in chain dynamics, and by multiple-quantum NMR for more detailed insights.

PB forms solid nanorods in the nanopores of the AAO. Filling kinetics experiments revealed the conditions under which the pore volume is completely filled and equilibrium is reached. At non-equilibrium stages, we observed strong deviations from the bulk-like entanglement-induced chain ordering, including much increased chain order and an inhomogeneous response, indicating possible layering effects. After the infiltration equilibrium was reached, the behavior was more homogeneous, but still significantly higher local chain order was detected. Moreover, MQ NMR data indicate a shift of Tg. All observed effects became more pronounced upon reduction of the pore diameter.

CPP 15.8 Mon 16:30 Poster C

Miniemulsion Polymerization Reactions Observed by Time-Resolved Xe-129 NMRR — •Mathis Düwel, Nicolas Vogel, Clemens Weiss, Katharina Landfester, Hans W. Spiess und Kerstin Münnemann — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

In the last years, Xe-129 NMR has found many applications in material science and medicine because of two useful properties of Xenon atoms in NMR: their sensitivity to their environment due to their highly polarizable electron cloud, even without the need for covalent bonds, and the ability of being hyperpolarized. Here, Xe-129 NMR is used in the online monitoring of polymerization reactions. The method allows for the online monitoring of polymerization by reporting quantitatively the composition of the reaction mixture by the chemical shift of hyperpolarized Xe. The hyperpolarized gas is brought into contact with the reaction mixture in an NMR tube in a 7 T-NMR spectrometer by the use of hydrophobic hollow-fibre membranes, allowing for the molecular dissolution of the hyperpolarized Xe into the miniemulsion. Repeated Xe-129 NMR measurements show the time-resolved polymerization process. The depolarized Xe is continuously replaced by the gas flow from the hyperpolarizer. Kinetic data for different reaction conditions (e.g., different initiators) has been determined from the chemical shift of the dissolved Xenon, allowing for the comparison with calorimetric data.

CPP 15.9 Mon 16:30 Poster C

Transport and high-pressure phase equilibria in mesopores — •Philipp Zeigermann, Muslim Dvoyashkin, Jörg Kärger, and Rustem Valiullin — Department of Interface Physics, University of Leipzig, Germany

Heterogeneous catalysis in high-pressure environments is a standard process in state-of-the-art industrial chemical synthesis. Micro- and mesoporous materials are widely used as hosts for the catalysts, while educts and products are delivered and removed under high pressure conditions. The supercritical state is here of particular interest because of its superior dynamical properties (low viscosity, no surface tension, high diffusivity).

Despite of its advantages in various applications, high-pressure phase equilibria in mesoporous host materials, and especially their interrelation with transport properties, are still poorly understood. Recently, it was shown that pulsed field gradient nuclear magnetic resonance spectroscopy (PFG NMR) is a particularly suitable tool to probe diffusion properties of sub- and near-critical fluids in mesopores.

A special NMR sample vessel has been constructed which permits to maintain pressures up to 200 bars. In this way it is possible to measure pressure-dependent self-diffusivities of organic compounds solved in supercritical solvents, e.g., in carbon dioxide in the bulk state as well as in the mesopores. Some preliminary results on molecular diffusivities at different conditions will be presented.

CPP 15.10 Mon 16:30 Poster C

Field-cycling-NMR: A new magnet design for reduced energy consumption — •Dirk Plendl, Alexei F. Privalov, and Franz Fujara — Institut für Festkörperphysik, TU Darmstadt, Hochschulstraße 6, 64289 Darmstadt

Field-cycling-NMR is an establiched method for the investigation of field dependent spin phenomena, like relaxation dispersion, polarization transfer, enhanced NQR etc. In contrast to normal NMR, the magnetic field in a field-cycling experiment is switched between several distinct levels within milliseconds. This can only be achieved with specially designed, low inductive magnets.

Today, nearly all FC-spectrometers utilize air core coils made of copper or silver. Producing strong magnetic fields with normal-conducting magnets results in a large energy dissipation (tens of kW) so that the maximum field strength is limited by the amount of heat that can be extracted by the cooling system.

We present a new magnet design for fast field-cycling-NMR which uses a magnet with an iron core for field amplification, thus generating the same field with significantly reduced energy consumption and system complexity [1].

[1] D. Plendl, M. Fujara, A. F. Privalov, F. Fujara, J. Mag. Res. 198 (2009) 183-187

CPP 15.11 Mon 16:30 Poster C

A spatially resolved mechanical field cycling relaxometer — •Michael Ditter[1], Holger Stork[1,3], Achim Gädke[1,4], Franz Fujara[1], Beatrice Schuster[1,2], Christina Trautmann[2], and Reinhard Neuman[2] — [1]Institut für Festkörperphysik, TU Darmstadt, Hochschulstr. 6, Darmstadt — [2]GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt — [3]National des Champs Magnétiques Intenses, r. d. Martyrs, Grenoble — [4]School of Engineering and Computer Science, Victoria University, Kelburn Parade, Wellington

Recently a new method for the spatially resolved characterization of heavy ion irradiated crystals using static field gradient NMR was developed [1]. With this method it is possible to measure one-dimensional spin-lattice relaxation rate profiles with a spatial resolution in the order of $10\,\mu$m. In the meantime the spectrometer has been further improved and the method expanded to conduct frequency and temperature dependent measurements. For field cycling NMR the probe is moved inside the stray field of a superconducting magnet. Due to the strong magnetic field gradient only the nuclei within a thin excited slice are in resonance, allowing spatial resolution. It is possible to utilize fields between 6.3 and 0.008 T. The positioning system is capable of achieving switching times of less than 5 s. The accessible sample temperature ranges from RT to 500 K. The relaxometer will be used for spatially resolved spin-lattice relaxation dispersion experiments of swift heavy ion irradiated ionic crystals.

[1] Stork H, Hamburger A, Gädke A, Fujara F and Schwartz K 2008 J. Phys.: Condens. Matter 20 275236

CPP 16: Nuclear Magnetic Resonance: Frontiers and Applications

Time: Tuesday 13:45–16:15 Location: H48

CPP 16.1 Tue 13:45 H48

Probing the Assembly and Dynamics of Graphene-Inspired Molecular Wires by Solid-State NMR Spectroscopy — •Michael Ryan Hansen, Robert Graf, Daniel Sebastiani, and Hans-Wolfgang Spiess — Max Planck Institute for Polymer Research

Molecular wires based on polycyclic aromatic hydrocarbons (PAHs) are apromising class of materials for future applications in nano-scale electronic devices. Critical for the performance of such wires are their molecular assembly, which on the NMR length and time scales translates into the local packing arrangement, molecular dynamics, and pitch angle(s) between successive molecules. Here, we show that solid-state NMR in combination with MD and ab-initio calculations can provide unique information with respect to these structural features. To illustrate this we examinine two perylene tetracarboxydiimides (PDIs) with different side chains attached and a larger triangular-shaped PAH. Specifically, we measure 1H chemical shifts using fast MAS and their spatial connectivities through 2D 1H-1H DQ-SQ correlation spectra and probe the molecular dynamics via 1H-13C heteronuclear dipolar couplings. To support the experimental findings we have performed CPMD-NMR calculations to reveal the effects of packing on the 1H chemical shifts for the PDIs, including an estimate of the line broadening due to local disorder. This provides a series of finger prints for different pitch angles between neighboring molecules, that are closely related to the electronic conduction properties of the supramolecular stacks.

CPP 16.2 Tue 14:00 H48

NMR studies of benzene mobility in microporous metal-organic framework MOF-5 — •Stefan Hertel[1], Saeed Amirjalayer[2], Markus Wehring[1], Rochus Schmid[2], and Frank Stallmach[1] — [1]Universität Leipzig, Fakultät für Physik und Geowissenschaften, Deutschland — [2]Ruhr-Universität Bochum, Fakultät für Chemie und Biochemie, Deutschland

Microporous metal-organic frameworks (MOF) are crystalline coordination polymers with regular three dimensional pore networks. These pore networks enable adsorption and diffusion of guest molecules. Molecular Dynamics (MD) simulations show that benzene has a liquid-like mobility inside the pores of MOF-5. Nuclear Magnetic Resonance (NMR) methods allow experimental access to guest mobilities inside such pore networks. This report presents the results of pulsed field gradient NMR (PFG NMR) self-diffusion measurements of benzene adsorbed in MOF-5. In these experiments multi-exponential spin echo decays were observed, which are usually caused by different phases of self-diffusion. These different phases of benzene mobility were unexpected for diffusion of molecules inside an isotropic framework and have to originate in the host-guest and guest-guest interaction. By modern diffusion-relaxation correlation spectroscopy (DRCOSY) translational self-diffusion and microscopic relaxation behavior were correlated. Together with magic angle spinning (MAS) NMR spectroscopy these investigations reveal that the faster component of the diffusion coefficients can be assigned to diffusion inside the porous crystal structure of MOF-5.

CPP 16.3 Tue 14:15 H48

Exploring the limits to spatially resolved NMR — Achim Gädke[1,2] and •Nikolaus Nestle[1,3] — [1]TU Darmstadt, Institute of condensed matter physics, Germany — [2]Present adress: Victoria University of Wellington, New Zealand — [3]Present adress: BASF SE, GKC/R, Ludwigshafen, Germany

Recent advances in MRI have demonstrated resolutions down to 1 μm. Magnetic resonance force microscopy has the potential to reach sensitivity for single nuclear spins. Given these numbers, in vivo imaging of single cells or even biomacromolecules may seem possible. However, for in vivo applications, there are fundamental differences in the contrast mechanisms compared to MRI at macroscopic scales as the length scale of of molecular self-diffusion exceeds that of the spatial resolution on the NMR time scale. Those effects - which are fundamentally different from the echo attenuation in field gradient NMR - even may lead to general limitations on the spatial resolution achievable in aqueous systems with high water content. In our contribution, we explore those effects on a model system in a high-resolution stray-field imaging setup. In addition to experimental results, simulations based on the Bloch-Torrey equation will be presented.

CPP 16.4 Tue 14:30 H48

Polymers under mechanical stress- an NMR investigation — •Ute Böhme[1], Bo Xu[2], Johannes Leisen[2], Haskell W. Beckham[2], and Ulrich Scheler[1] — [1]Leibniz Institute of Polymer Research Dresden — [2]Georgia Institute of Technology, Atlanta, Georgia

Low-field NMR using permanent magnets in Halbach arrangements permit NMR investigation without the limits present in high-field NMR. The lower field in conjunction with confined stray field permit the application of NMR, in particular relaxation NMR in a stretching apparatus and a rheometer [1,2]. Crystalline and amorphous fraction of semi-crystalline polymers are distinguished by their transverse relaxation times. Upon mechanical load the relaxation times of the amorphous fraction changes as seen in in-situ measurements on polypropylene rods. During the formation of a neck the crystalline fraction becomes more prominent.

[1] S. Kahle et.al., KGK- Kautschuk Gummi Kunststoffe 61 (2008), 92.

[2] G. Mazzanti et.al., J. Am. Oil Chem. Soc. 85 (2008), 405.

CPP 16.5 Tue 14:45 H48

Segmental Order in Polymer Networks — •Jens-Uwe Sommer — Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, 01069 Dresden, Germany

Polymer networks are structurally and topologically disordered soft solids. We consider orientation order of chain segments in polymer networks to relate NMR-experiments with molecular models of polymer networks [1,2]. We derive a general relation between segmental order and local forces acting on a chain under external constraints. Using this result, we consider good solvent conditions and we show that the solvent plays a crucial role for the tensor order parameter. In particular, we show that the tensor order parameter decreases due to excluded volume interactions. Using analytical results and scaling arguments we derive a universal behavior for the order parameter with respect to the equilibrium degree of swelling which can be experimentally verified [2]. In the light of these observation we discuss several microscopic models of network swelling. Using the general relation between local forces on chain bonds and the tensor order parameter we further discuss possible observations on structurally regular networks such as obtained recently in experiments based on force-balance arguments, as well as the role of entanglements.

[1] J.-U. Sommer and K. Saalwächter, European Phys. J. E 18 (2005) 167-182

[2] J.-U. Sommer, Walter Chassé, Juan López Valentín, and Kay Saalwächter, Phys. Rev. E 78, 051803 (2008)

CPP 16.6 Tue 15:00 H48

Ultrafast velocity-mapping in microfluidic setups — •Eva Paciok, Andrea Amar, Federico Casanova, and Bernhard Blümich — ITMC, RWTH Aachen University, Germany

NMR in combination with designated rf coils has proven to be a powerful tool for the investigation of microfluidic setups, e.g. microreactors, micromixers and fluid drops, since it has the potential to reveal both spectroscopic, spatial and velocity information non-invasively. Despite the high spatial resolution NMR offers, the temporal resolution of NMR imaging and velocity mapping experiments in microfluidics has been low so far, because the application of ultrafast NMR velocity mapping methods to microfluidics has failed. These methods are based on multi-echo generation give rise to problems concerning magnetic field inhomogeneities (EPI), rf field inhomogeneities (PGSE-RARE) and velocity/acceleration limitations (EPI and PGSE-RARE).

In this work, we exploit the advantages of the FLIESSEN (Flow Imaging Employing a Single Shot ENcoding) pulse sequence, a new ultrafast RARE-based imaging and velocity mapping method. An adjusted phase encoding strategy and a frequent update of velocity encoding during the multi-echo train makes FLIESSEN highly resilient to field inhomogeneities and velocity/acceleration effects. The performance of this technique is demonstrated on acetone flow in a microstructured phantom. Using FLIESSEN and a surface rf coil, high-fidelity 2D velocity maps were acquired within seconds.

CPP 16.7 Tue 15:15 H48

Structural characterization of lyotropic lamellar phases by NMR spectroscopy — Bruno Medronho[1,2], Maria G. Miguel[1], Ulf Olsson[2], and •Claudia Schmidt[3] — [1]Department of Chemistry, University of Coimbra, 3004-535 Coimbra, Portugal — [2]Physical Chemistry, Center of Chemistry and Chemical Engineering, Lund University, Box 124, 221 00 Lund, Sweden — [3]Department of Chemistry, University of Paderborn, Warburger Str. 100, 33098 Paderborn, Germany

The lyotropic lamellar L_α phase is usually considered to consist of stacks of extended parallel layers. However, the application of shear may lead to defect structures consisting of close-packed multilamellar vesicles, also known as onions. Furthermore, it has been suggested that an intermediate structure of multilamellar cylinders occurs during the transformation from layers to vesicles. In this contribution we will give an overview on what kind of structural information can be obtained by deuterium NMR spectroscopy applied in situ under shear. It will be shown how different structures can be distinguished, how onions can be formed and destroyed by the application of shear and how the onion size can be measured on the basis of an NMR line shape analysis.

CPP 16.8 Tue 15:30 H48

Complete NMR spectral assignment in gibbsite by first-principle calculations — •Anastasia Vyalikh and Ulrich Scheler — IPF Dresden, Hohe Str. 6, D-01069 Dresden, Germany

The structure of the mineral gibbsite is often considered as a representative of many alumino-silicate clay minerals, and therefore we use it in the present study as a model compound to establish the suitability of the computational method. Here we apply a gradient-corrected DFT method with a plane-wave basis set to assign the crystallographically distinct Al sites in gibbsite and to relate them to the hydroxide network. The experimental observation is based on high-resolution solid-state 27Al NMR and 1H CRAMPS (combined rotation and multipulse spectroscopy) data. On the basis of DFT calculations, the 1H CRAMPS signals have been attributed to six symmetry independent hydrogen atoms and ascribed to two distinct types associated with intralayer and interlayer hydrogen bonds. The 27Al NMR spectrum shows signals for octahedral aluminium only, however with two distinguished signals. The correlation between experimental and theoretical NMR parameters demonstrates that the character of the hydrogen bonds formed by the hydroxide ions is responsible for the structural differentiation of Al sites. That is, the Al-I site (CQ=4.2 MHz) is surrounded by the OH-groups particiating in 4 intralayer and 2 interlayer hydrogen bonds, while the Al-II site (CQ=2.4 MHz) is coordinated by the hydroxides, 2 of which point towards the intralayer cavities and 4 OH-bonds are aligned towards the interlayer gallery.

CPP 16.9 Tue 15:45 H48

Heparin-polynitroxide derivatives: biocompatible polarizing agents for dynamic nuclear polarization (DNP) — •Björn C. Dollmann[1], Andrei L. Kleschyov[2], Vasily Sen[3], Valery Golubev[3], Laura Schreiber[4], Kerstin Münnemann[1], and Dariush Hinderberger[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Second Department of Medicine, Johannes Gutenberg University, Mainz, Germany — [3]Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, Russia — [4]Johannes Gutenberg University Medical Center, Mainz, Germany

A versatile and biocompatible class of spin-labeled macromolecules was investigated by electron spin echo-detected (ESE) electron paramagnetic resonance (EPR), continuous-wave (CW) EPR, double electron-electron resonance (DEER) and dynamic nuclear polarization (DNP). These heparin macromolecules could be utilized for *in vivo* magnetic resonance imaging (MRI DNP enhanced) and EPR imaging (EPRI). The distance distributions of the spin labels were measured and compared with the crystallographic structure of heparin. All presented heparin-polynitroxides show reasonably high ^1H DNP enhancement factors up to $E = -108$. The heparin-polynitroxides intrinsically feature high dipolar electron spin-electron spin coupling frequencies ν_{dd}. Together with the finding that the best ^1H-signal enhancements are found in the low concentration region, this proves the influence of the anisotropic electron spin distribution on DNP in liquids at room temperature.

CPP 16.10 Tue 16:00 H48

Structure of Phage SPP1 Head-to-Tail Connector Reveals Gating Mechanism for DNA Ejection: an EM and NMR study — Matthieu Gallopin[1], Sophie Lhuillier[2], Bernard Gilquin[1], Sandrine Brasilès[2], Elena Orlova[3], Joël Couprie[1], Paulo Tavares[2], and •Sophie Zinn-Justin[1] — [1]Laboratoire de Biologie Structurale et Radiobiologie, iBiTec-S, CEA Saclay, Gif-sur-Yvette, France — [2]Unité de Virologie Moléculaire et Structurale, UMR CNRS 2472, UMR INRA 1157 and IFR 115, Gif-sur-Yvette, France — [3]Department of Crystallography, Birkbeck College, University of London, London, UK

Understanding the principles that govern macromolecular assembly is a current challenge for biochemists, molecular biologists, and structural biologists. Assembly of bacterial virus (bacteriophages) particles is a highly suitable system to investigate the molecular mechanisms that support efficient formation of a complex macromolecular machine and its function. A large number of phages and eukaryotic viruses use a portal system to control genome entry and exit from their capsids. The portal and head completion proteins form the viral head-to-tail connector. The pseudo-atomic structure of the complete closed connector of tailed bacteriophage SPP1 was determined (Lhuillier et al., PNAS 2009). Opening of the connector and DNA ejection from virions was reproduced in vitro by adding the host purified receptor YueB. These achievements recommend SPP1 as an excellent system to investigate the structural organization and dynamics of the viral DNA gatekeeper.

CPP 17: Interfaces and Thin Films I

Time: Tuesday 9:30–12:45 Location: H39

Topical Talk CPP 17.1 Tue 9:30 H39

Surviving Structure in Colloidal Suspensions Confined from 3D to 2D — Yan Zeng[1], Stefan Grandner[2], Sabine Klapp[2], and •Regine von Klitzing[1] — [1]Stranski-Laboratorium, Institut für Chemie, TU Berlin — [2]Institut für Theoretische Physik, TU Berlin

Due to miniaturization the question arises how geometrical confinement in thin films affects the structure and dynamics of colloidal suspensions. The film thickness is between 5 - 150 nm and therefore on the same mesoscopic length scale as the distance between colloidal particles. For studying the interaction with the thin film, either a Colloidal Probe AFM or a Thin Film Pressure Balance (TFPB) was used. The resulting structural (oscillatory) forces are characterized by their period, decay length and amplitude. We have proven experimentally the predictions of the Density Functional Theory (DFT) that the confinement does not affect the characteristic lengths of the colloidal dispersion. Our results show that the wavelength obtained by the structure peak from neutron or x-ray scattering experiments at the volume phase is equal to the period of the force oscillation in the film [1,2]. In other word, the average polymer or particle distance, i.e. the concentration remains the same. The effect of different parameters like ionic strength [3] and influence of the properties of the confining surfaces (charge, softness) are shown. [3]. [1] D. Qu, J.S. Pedersen, S. Garnier, A. Laschewsky, H. Möhwald, R. v. Klitzing Macromolecules (2006) 39 7364. [2] S. Klapp, Y. Zeng, D. Qu, R. v. Klitzing Phys. Rev. Letters (2008) 100 118303. [3] S. Grandner, Y. Zeng, R. v. Klitzing, S.H.L. Klapp, J. Chem. Phys. (2009) on Web.

CPP 17.2 Tue 10:00 H39

Soft Colloidal Probe AFM - A New Method for the Investigation of Adhesion and Contact of Soft Surfaces — •Johann Erath, Stephan Schmidt, Petra Zippelius, and Andreas Fery — Universität Bayreuth, 95440 Bayreuth, Germany

We introduce a novel approach for AFM based adhesion measurements which combines the advantages of the JKR-apparatus and AFM-force-spectroscopy. We create a defined microscopic contact by using a soft colloidal probe made of Polydimethylsiloxane. This allows in-situ determination of the contact area as a function of applied load and elastic properties of the sytem. Hence, similar to the JKR-apparatus, adhesion energies can be determined from a fit of a whole set of data of well-defined contact areas and load forces. Besides tests on model systems, where we can clearly characterize contributions of capillary forces, hydration forces and hydrophobic interactions, this technique makes a broader range of systems and scientific issues accessible. In this presentation we focus on the lower limit of elastic constants, where the probes will approach typical values for soft biological materials like cells and thus provide elasticity matched partners for adhesion measurements.

CPP 17.3 Tue 10:15 H39

Solvent evaporation induced ordered array of colloidal particles — •Mottakin M. Abul Kashem, Suttipong Wannapaiboon, Adeline Buffet, Jan Perlich, Rainer Gehrke, and Stephan V. Roth — Hasylab at DESY,Notke Str.85, 22607 Hamburg

Solvent evaporation during drying of a colloidal film or a droplet on a solid substrate can introduce ordering in the final dried film [1]. During solvent evaporation in a droplet of colloidal suspension the colloidal particles are transported towards the periphery while the contact-line among substrate, ambient air and droplet moves towards the center of the droplet. During these two simultaneous processes one or two dimensional ordered nano and microstructures can be spontaneously formed based on the surface free energy of the substrate. Besides, sedimentation of the colloidal particles and capillary forces during drying also play an important role on the formed 3-dimensional ordered structures. In this present investigation, we show the influence of substrate surface on the nano and microstructures formed during solvent evaporation in colloidal droplets containing polystyrene latex microspheres. The arrangement of the nano and microparticles has been investigated and imaged by using optical microscopy, atomic force microscopy (AFM) and grazing incidence small-angle X-ray scattering (GISAXS).

[1] Roth et al., Appl. Phys. Lett. 91, 091915 (2007)

CPP 17.4 Tue 10:30 H39

Thermal stability of spin-coated and sprayed colloidal PS-films — •Gerd Herzog[1,2], Adeline Buffet[2], Mottakin M. Abul Kashem[2], Rainer Gehrke[2], Peter Müller-Buschbaum[3], Jan Perlich[2], Matthias Schwartzkopf[2], Wilfried Wurth[1], and Stephan V. Roth[2] — [1]Institut für Experimentalphysik der Universität Hamburg, Luruper Chaussee 149, D-22761 Hamburg, Germany — [2]HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany — [3]Physik-Department E13, TU München, James-Franck-Str. 1, D-85748 Garching, Germany

Installation of large scale colloidal nanoparticle thin films is of great interest in sensor technology or magnetic storage [1]. Among the methods used are dip-coating, spin-coating and spray deposition. Often, such devices are operated at elevated environmental or thermal conditions. In our study presented here, we investigated in-situ the effect of heat treatment on the structure of differently prepared colloidal solutions of polystyrene nanospheres by grazing incidence small angle x-ray scattering (GISAXS) and optical microscopy. We used two routes to install large scale coatings on silicon wafers, namely spin-coating and spray-coating of colloidal polystyrene (PS) nanospheres, having different outer end groups. Our first results indicate that thermal annealing in the vicinity of the glass transition temperature of pure PS leads to a rapid loss in the long range order in spin-coated films. Our model uses an increased mobility of the nanoparticles to explain this behaviour [2]

[1] Bigioni et al., Nature Materials 5, 265-270 (2006) [2] Herzog, Diplomarbeit, Universität Hamburg (2009)

15 min. break

CPP 17.5 Tue 11:00 H39

Delayed Coalescence of Sessile Droplets with Different but Miscible Liquids — •Stefan Karpitschka and Hans Riegler — Max-Planck-Institut für Kolloid- und Grenzflächenforschung, 14476 Potsdam, Germany

Due to capillary forces two sessile droplets of miscible liquids will fuse when they get in contact with each other. Usually the droplet fusion proceeds very fast, delayed mostly by viscous forces. However, quite unexpected, it was observed recently [1] that the coalescence of sessile droplets of completely miscible liquids can be delayed up to minutes. After first contact, the droplets remain separated by a thin liquid neck and push each other across the substrate before they finally merge.

It is assumed [1] that the coalescence is delayed by a marangoni convection through the thin film connecting the drops. This suggests that the effect is quite common. Meanwhile it could also be modeled in the framework of phase field formalism and lubrication approximation [2]. The delayed coalescence may be relevant for technical applications, e.g. in the field of microfluidics.

We present new results from experiments addressing the influence of the liquid properties on the coalescence behavior. A sharp transition from fast to delayed coalescence is observed when the difference in surface tensions exceeds approximately 4 mN/m. Other parameters like absolute surface tensions, viscosities, and contact angles have been varied to generate a phase diagram of coalescence.

[1] H. Riegler et al., Langmuir 24, 6395-6398, 2008.

[2] R. Borica et al., Phys. Fluids, submitted.

CPP 17.6 Tue 11:15 H39

The Softer the Better: Fast Condensation on Soft Surfaces — Mordechai Sokuler[1,2], •Günter K. Auernhammer[1], Marcel Roth[1], Chuanjun Liu[1,2], Elmar Bonaccurso[1], and Hans-Jürgen Butt[1] — [1]MPI Polymer Research, Mainz, Germany — [2]Center of Smart Interfaces, TU Darmstadt, Germany

Condensation on soft elastic surfaces differs significantly from condensation on hard surfaces [1]. On polymeric substrates with varying cross-linking density, we investigate the nucleation and the growth of condensing water drops. Surface roughness and apparent contact angle are shown to be very similar on all surfaces. The surfaces differ in the elastic module and viscosity. With increasing softness of the substrates, we find (1) increasing nucleation density, (2) longer relaxation times for drop shape equilibration after merging of two drops, and (3) prevention of merging on very soft surfaces. These effects lead to higher surface coverage and overall condensed volume on soft surfaces.

[1] M. Sokuler et al. Langmuir (2009), DOI: 10.1021/la903996j

CPP 17.7 Tue 11:30 H39

Au-Nanoparticle on the Water Surface — •Volker Schön[1], Patrick Huber[1], Philip Born[2], and Tobias Krauss[2] — [1]Saarland University, 66123 Saarbrücken, Germany — [2]Leibniz-Institut für Neue Materialien gGmbH, 66123 Saarbrücken, Germany

This contribution has been withdrawn.

CPP 17.8 Tue 11:45 H39

Surface plasmon induced structuring of azobenzene thin polymer films — •Nataraja Sekhar Yadavalli[1], Tobias König[2], and Svetlana Santer[3] — [1]Department of Microsystems Engineering (IMTEK), Freiburg — [2]Freiburg Institute for Advanced Studies (FRIAS), Freiburg — [3]Department of Experimental Physics, Potsdam

There is a strong demand on methods for precise manipulation of nano-objects on surfaces. Recently we report on a phenomenon observed with a certain type of thin polymer films, suggesting that the substrate by itself can induce motion of adsorbed objects (Santer, 2006). The proposed mechanism of motion is based on a dynamically fluctuating force field, emerging during topography switching. It results in competing surface forces acting on the particle, which leads to a motion and repositioning of the particle. In this work, we choose UV-illumination for changing the topography of photosensitive thin polymer films. Here we present azo thin films (Seki, 2007) with integrated optically active elements supposed to support and steer the response of polymer films to external illumination. The nano-scale metallic structures were fabricated on glass substrate using Au/Ag by colloidal lithography. During irradiation the surface plasmon waves are generated on a metallic mask, which results in printing of near field intensity distributions into topography with the pattern size below the diffraction limit. We found that the topography can be driven reversible. We examined the influence of size of the metallic patterns. The results are confirmed by FDTD simulations and compared with imprints of photolithographic mask.

CPP 17.9 Tue 12:00 H39

Single molecule diffusion in liquid crystals — •Martin Pumpa and Frank Cichos — Molecular Nanophotonics Group, University of Leipzig

Liquid crystals show a strong orientational order along a certain director, while lacking spatial order of their centers of mass. For uniaxial molecules the orientational properties lead to an anisotropy in the optical properties of the material and the mobility as well.

Recent studies have focused on the diffusion of macroscopic particles in the matrix of the liquid crystal. In case of macroscopic probes the director structure around such colloids is strongly altered due to anchoring effects at the particle surface, leading to distortions in the orientation of the liquid crystal and therefore to an rotational contribution to the measured drag forces. Such effects are absent in the study of single molecule diffusion in liquid crystals. We thus present results on the translational and rotational diffusion of single fluorescent probe - molecules in the nematic phase of 5CB and the smectic phase of 8CB. We used single molecule tracking to determine the anisotropy of translational diffusion of PDI molecules and time resolved fluorescence microscopy to observe their rotational behavior. We are able to relate our results directly to the director structure of the liquid crystalline phases by means of polarization contrast microscopy.

CPP 17.10 Tue 12:15 H39

Single Molecule Orientation and Binding on Surfaces — •Stefan Krause[1], Danny Kowerko[1], Richard Börner[2], Christian Hübner[2], and Christian von Borczyskowski[1] — [1]Chemnitz University of Technology D-09107 Chemnitz, Germany — [2]University of Lübeck, D-23538 Lübeck, Germany

Orientation of molecules at a solid interface is an important issue for the modification of surfaces, synthesis, catalysis or photovoltaic. Optical single molecule detection is one of the powerful tools to determine the orientation of even a single molecule via measurement of the orientation of the electric dipole transition. One of the most suited dye molecules to study single molecule orientation is the perylene diimide-type system (PDI) featuring high quantum efficiency and photo stability. Here we present three methods to determine single molecule orientation of PBI selectively bonded via pyridyl groups to silicon dioxide [1]. Using microscope objectives with high numerical aperture allows for the direct determination of the timedependent three dimensional orientation of the transition dipole and the molecule axis [2]. In the second method we directly follow via two detection channels the polarisation of single molecule emission. The third method makes use of the orientation dependent distribution of fluorescence intensities of single molecules and the comparison to calculated distributions.

[1] D. Kowerko, J. Schuster, C. von Borczyskowski, 2009. Molecular Physics, 107, 1911- 1921

[2] J. Hohlbein, C. G. Hübner, 2008. Journal of Chemical Physics, 129, 094703

CPP 17.11 Tue 12:30 H39

Analysis of heterogeneous diffusion in ultra-thin liquid films via single particle tracking — •Ines Trenkmann, Daniela Täuber, Michael Bauer, and Christian von Borczyskowski — Chemnitz University of Technology, Institute of Physics, Germany

It has been well known for some years that the dynamical behavior of tracers in ultra-thin liquid films differs from the behavior in a bulk liquid. In previous studies of single dye diffusion in TEHOS-films (deposited on Si wafers with a thermally grown oxide layer) we could show that single particle tracking can reveal heterogeneous behavior of the used tracers [1]. Thereby the diffusion is influenced by dynamic and static heterogeneities [2]. The first ones are caused by changes between layers with distinct diffusion coefficients and the influence of the hydrodynamic boundary conditions. The latter are caused by surface heterogeneities, such as the inhomogeneous distribution of silanol groups on the silicon oxide surface. In recent studies we could show that the determined diffusion coefficients depend strongly on the applied evaluation method [3]. The determinations of the mean squared displacement just yield averaged diffusion coefficients. We are using short range diffusion coefficients from the analysis of scaled squared displacements at different time lags to obtain further information about the contributing heterogeneous components.

[1] Schuster, J., et al.: Eur. Polym. J. 40 (2004) 993

[2] Bauer, M., et al.: Diffusion Fundamentals 11 (2009) 70

[3] Trenkmann, I., et al.: Diffusion Fundamentals submitted

[4] Täuber, D.; et al.: Diffusion Fundamentals 11 (2009) 76

CPP 18: Interfaces and Thin Films II

Time: Tuesday 13:45–16:15 Location: H39

Topical Talk CPP 18.1 Tue 13:45 H39

Functional thin films based on polymer- and hybrid-nanostructures for photovoltaic applications — •Peter Müller-Buschbaum — TU München, Physik-Department LS E13, James-Franck-Str. 1, 85747 Garching

Conducting photoactive polymers offer fascinating new possibilities with respect to energy research applications such as photovoltaics (PV). In the organic photovoltaics (OPV) approach both parts of a thin film, the n- and p-type material, are made from such conjugated polymers. In a hybrid approach typically the p-type conducting polymer is in contact with a metal oxide as for example titania. For both types of PV systems, the tailoring of the interface morphology between n- and p-type materials is essential. The small exciton diffusion length in conducting polymers causes a need for domain sizes on that scale, thereby resulting in the bulk heterojunction approach. Grazing incidence small and wide angle scattering allow for a determination of this inner structure, which is the essential key for tailoring morphologies. In OPV model systems the influence of blend ration [1] and prost production treatments [2] on both, device performance and morphology, are discussed.

[1] Ruderer, Müller-Buschbaum et al.; Chem. Phys. Chem. 10, 664-671 (2009)

[2] McNeill, Müller-Buschbaum, et al.; Adv. Funct. Mat. 19, 3103-3111 (2009)

CPP 18.2 Tue 14:15 H39

Formation of lateral structures in thin diblock copolymer films by vapor treatment — Alessandro Sepe[1], Peter Cernoch[2], Petr Stepanek[2], Detlef-M. Smilgies[3], Stephan V. Roth[4], Andreas Timmann[4], and •Christine M. Papadakis[1] — [1]TU München, Physikdepartment E13, Garching — [2]Inst. Macromolecular Chemistry, Prague, Czech Republic — [3]Cornell University, Ithaca NY, USA — [4]HASYLAB at DESY, Hamburg

Exposure of block copolymer thin films to solvent vapor allows to control the orientation of the mesostructure with respect to the film surface. Using real-time, in situ grazing-incidence small-angle X-ray scattering (GISAXS), we have investigated the structural changes in thin films of lamellae-forming poly(4-octylstyrene-b-butylmethacrylate) [1] during exposure to hexane and cyclohexane vapor.

We have varied the initial film thickness and have found that, in all cases, a lateral structure is created. However, both, the kinetics of structure creation and the final repeat distance depend strongly on the film thickness and on the solvent chosen. Instabilities are observed during the first few minutes of vapor exposure in the thicker films, whereas the behaviour is continuous in the thinner film.

1. P. Cernoch, P. Stepanek et al., Eur. Poly. J. 43, 1144 (2007)

CPP 18.3 Tue 14:30 H39

Creating Nanostructures with Supramolecular Copolymers: A DFT-based Monte Carlo Approach — •Kostas Daoulas[1], Anna Cavallo[2], Roy Shenhar[3], and Marcus Müller[1] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany — [2]Dipartimento di Fisica "E.R. Caianiello", Universitá degli Studi di Salerno, Italy — [3]Institute of Chemistry and the Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, Israel

Designing assembling molecular systems capable of changing the morphology in response to external stimuli is important for nanotechnology related applications. We develop a density functional theory based Monte Carlo approach for studying assembling supramolecular, "living", copolymer systems in the bulk and in thin films. Here, we consider a system consisting of A and B monomers, where all A monomers are permanently bonded into n blocks, connected irreversibly at one end to a short B block so that irreversible AB diblocks are formed. The remaining B monomers can reversibly associate into linear chains, with each other as well as with the B terminus of the diblock; thus the spectrum of the different molecular species consists of B homopolymers, AB diblocks, and ABA triblocks. We discuss representative phase diagrams as a function of the A/B block ratio, the A/B monomer incompatibility, and the strength of the B-species association energy. The interplay between the morphology and system stoichiometry is highlighted. We conclude by considering the perspectives of directing the assembly of living copolymers using patterned substrates.

CPP 18.4 Tue 14:45 H39

Bundle Formation in Polyelectrolyte Brushes Caused by Divalent Ions — •Heiko Ahrens[1], Jens-Uwe Günther[1], Stephan Förster[2], and Christiane A. Helm[1] — [1]Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Str. 6, D-17489 Greifswald, Germany — [2]Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, D-20146 Hamburg, Germany

Monolayers from amphiphilic block copolymers consisting of a fluid hydrophobic and a polyelectrolyte part are studied with X-ray reflectivity and Grazing Incidence Diffraction. The concentration of divalent cations (Ca2+, Sr2+) is varied between 0.001 and 1 mM. At 0.001 mM the brush thickness is almost constant resembling the osmotic brush phase (brush thickness almost 50 % of contour length), at 1 mM the brush shrinks and the thickness scales with the molecular area with an exponent -0.5 (brush thickness as small as 20% of the contour length). Always, between two and four chains form a bundle, independent of salt concentration. For concentrations between 0.003 and 1 mM, the peaks are very weak, suggesting only small fractions of the chains form bundles. At 0.001 mM, the peak is stronger, similar to findings with monovalent ions in solution. We conclude that the divalent ions form links between polyelectrolyte chains, which is very different from monovalent ions. For monovalent ions, the aggregation number varies due to a balance between long-ranged electrostatic repulsion, whose range and amplitude is decreased on salt addition, and a short-ranged attraction presumably due to hydrophobic forces (J.U. Günther et al., PRL 2008, 101 (2008) No. 258303).

CPP 18.5 Tue 15:00 H39

Single polyelectrolyte layers adsorbed at high salt conditions: polyelectrolyte brush domains coexisting with flatly adsorbed chains — •Stephan Block and Christiane A. Helm — Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Str. 6, D-17489 Greifswald, Germany

AFM is used to measure the surface forces and to image sodium poly(styrene sulfonate) (PSS) layers physisorbed from 1 M NaCl solution on different length scales within one experiment. Domains of PSS brushes coexist with flatly adsorbed PSS. For degree of polymerization N = 380, the brush area fraction 6 %. With increasing degree of polymerization, brush area fraction and domain size increase, while the domain radii range from 50 nm up to 1500 nm. Laterally homogeneous brush layers are found for a degree of polymerization exceeding 1100. Colloidal probe technique reveals that the surface forces are a superposition of steric and electrostatic forces, their respective contribution is determined by the brush area fraction. A comparison with literature demonstrates that adsorbed PSS brushes show the same scaling behaviour as end-grafted PSS brushes. We develop a model for the adsorption of polyelectrolytes in which not the whole chain but only a fraction of the monomers adsorbs onto the surface. Thereby we show that partial adsorption can lead to stable conformations and calculate scaling laws for the fraction of adsorbed monomers and the distance between the chains dangling into solution.

CPP 18.6 Tue 15:15 H39

Polyelectrolyte Solutions Confined between Two Solid Surfaces — •Cagri Üzüm and Regine v. Klitzing — Stranski-Laboratorium für Physikalische und Theoretische Chemie - Institut für Chemie TU Berlin, Sekr. TC 9 Strasse des 17. Juni 124 D-10623 Berlin

Thin liquid films play an important role in macroscopic colloidal systems. Stability of a colloidal suspension -in which particles are dispersed in a liquid- is mainly dominated by the stability of the thin films seperating the dispersed particles.

In this contribution, liquid thin films of polyelectrolyte (PSS and PAMPS derivatives) solutions confined between two solid surfaces are studied. Colloidal Probe AFM is used to study the structure formation of aqueous polyelectrolyte solutions under geometrical confinement.

It was observed that AFM force measurements on the polyelectrolyte solutions lead to oscillatory force curves in a certain concentration range. These oscillatory curves can be used to study the interactions between the polyelectrolyte chains, which were described also by theoritical models. Concentration, type of the monomers and charge fraction of the polyelectrolyte chains determine the structuring [1]. In addition to those, effect of surfactant in the system, molecular weight and architecture of the polyelectrolyte chains on the structuring were investigated. Viscosity and conductivity measurements were taken for a better understanding of the phenomena.

[1] D. Qu, J.S. Pedersen, S. Garnier, A. Laschewsky, H. Möhwald and R. v. Klitzing. Macromolecules 39, 7364 (2006).

CPP 18.7 Tue 15:30 H39

Analysing the development of entanglements in spin coated films — •Julia Zabel and Alexander Blumen — Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg

As technological applications increasingly probe the nano scale and the importance of polymers in such devices rises, it becomes more and more important to understand the behavior of polymers confined to molecular lengthscales. Over the last years there has been a vast amount of experiments designed to understand the deviation of the properties of thin films from the bulk behavior. One can measure a film thickness dependence in such quantities as the glass transition temperature, the elastic modulus and relaxation times. But as varied as the experimental setups are the results. The often contradicting conclusions give rise to the suspicion that film preparation and annealing might play a large role in the outcome of the experiments. This is why we choose to research out-of-equilibrium films. In a toy model based on the spin coating process we simulate films of varying thickness and chain length. We then study their relaxation by analysing the polymers' conformation and entanglement over time. We discuss and compare different procedures to count entanglements, such as the determination of the self density, the so-called "packing model" and the Primitive Path Analysis. In this context we question whether reaching an equilibrium value for the polymer extension necessarily indicates that an equilibrium situation for the entanglements is reached.

CPP 18.8 Tue 15:45 H39

Stress relaxation during polymer brush swelling — Sebastian Lenz[1], Adrian Rühm[2], Rüdiger Berger[1], and •Jochen S. Gutmann[1,3] — [1]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, D-55128 Mainz (Germany) — [2]Max-Planck-Institut für Metallforschung, ZWE FRM-II / N-REX+, Lichtenbergstr. 1, D-85747 Garching bei München (Germany) — [3]Institut für physikalische Chemie, Johannes Gutenberg Universität, Jakob-Welder-Weg 10, D-55099 Mainz (Germany)

End-tethered polymer brushes can be used to create switchable surfaces. The properties of such surfaces are dependent on the solvent quality. We focused on the swelling behavior of poly-methylmethacrylate (PMMA) brushes as a model system. The aim of the presented work was to relate structural brush features in the collapsed/swollen state, such as the brush thickness and the adsorbed solvent fraction, to mechanical properties.

The structure of the polymer brush was measured in situ with Neutron Reflectivity (NR) as a function of solvent quality. Using scaling theories the effective polymer-solvent interaction parameters could be estimated from the NR results.

Preparing the PMMA brush directly on nanomechanical cantilever sensor arrays allowed us to perform surface stress experiments and relate the obtained mechanical results to the results obtained from NR. It was concluded that attractive polymer/polymer interactions relax towards zero reaching theta solvent conditions.

CPP 18.9 Tue 16:00 H39

Cross-linked Polymer Brushes — •Max Hoffmann[1,2], Michael Lang[1], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Hohe Strasse 6, 01069 Dresden, Deutschland — [2]Institut für Theoretische Physik, Technische Universität Dresden, 01069 Dresden, Deutschland

Cross-linked polymer brushes have gained increasing attention in recent years. However, up to now there is only little theoretical work done on this topic. Based on simulations of the bond fluctuation model, the cross-linking process will be introduced in detail. The simulation based percolation threshold induced by the cross-links is lower than the percolation threshold which is expected from the mean field gelation model. In order to understand the percolation behavior a new percolation model is developed which we call star-percolation model. As a coarse-grained model the star-percolation model contains core features of the cross-linking process of the polymer brush. Standard properties like the percolation threshold and the cluster size distribution as well as other static and dynamic properties of the cross-linked polymer brushes are discussed.

CPP 19: Organic Electronics and Photovoltaics I

Time: Tuesday 9:30–12:45 Location: H37

CPP 19.1 Tue 9:30 H37

Side chain variations on dicyanovinyl-oligothiophenes studied by photoinduced absorption spectroscopy: consequences for small molecule organic solar cells — •Hannah Ziehlke[1], Roland Fitzner[2], Christian Koerner[1], Egon Reinold[2], Peter Baeuerle[2], Karl Leo[1], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden — [2]Institut für Organische Chemie II und Neue Materialien, Universität Ulm

Oligothiophenes capped with electron-withdrawing dicyanovinyl groups (DCVnT) are promising candidates for applications in small molecule organic solar cells. These oligothiophene derivatives can act as electron donor in blend layers with C_{60}. Single heterojunction devices reach efficiencies above 4 %. The introduction of side chains as intermolecular spacer has little effect on the energetics and mainly influences the morphology of the evaporated thin film. In addition, the distance between donor and acceptor molecules and thus the energy transfer and charge separation at the interface can be controlled. The energetic and dynamic properties of the long lived photoexcitations in pristine and blend layers can be obtained by photoinduced absorption spectroscopy (PIA). We here characterize of DCV3T with zero, two, and four alkyl chains (Methyl and Butyl) via PIA spectroscopy complemented with morphological studies. Our results indicate that the energy transfer process at the heterojunction is more efficient for smaller spatial distances between donor and acceptor molecules.

CPP 19.2 Tue 9:45 H37

New multiwall molecular organic nanotubes — •Maren Rastedt[1], Frauke Kutscher[1], Okko Frey[2], Rüdiger Beckhaus[2], Christian Maibohm[3], and Katharina Al-Shamery[1] — [1]University of Oldenburg, Physical Chemistry 1, Germany — [2]University of Oldenburg, Inorganic Chemistry, Germany — [3]NanoSYD, Sonderborg, Denmark

Nanotubes can be described as the newest star in the evening sky of nanotechnology. Since the discovery of carbon nanotubes , this nanostructure has grasped the mind of many. This structure has many application possibilities ranging from liquid and gas storage to microelectronics and sub wavelength optical components and fibers. In our presentation we will give an introduction to multiwall nanotubes made from Tetrabenzofluorene(Tbf)-derivates. These Tbf-nanotubes have attracted interest because of their many properties, e.g. crystallization and waveguiding. Our nanotubes are prepared by the elegant and simple process of template assisted assembly. The assembly process will be presented together with specific properties of different Tbf-nanotubes. By changing growth parameters in the assembly process we have a method for probing fundamental questions and properties of our nanotubes. One future application of our nanotubes could be as an active element in a photovoltaic device.

CPP 19.3 Tue 10:00 H37

Radical Molecular Wires — •Georg Heimel[1], Egbert Zojer[2], Lorenz Romaner[3], Jean-Luc Brédas[4], and Francesco Stellacci[5] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Germany — [2]Institut of Solid State Physics, Graz University of Technology, Austria — [3]Chair of Atomistic Modeling and Design of Materials, University of Leoben, Austria — [4]School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, USA — [5]Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, USA

The technological relevance and the functionality of semiconducting materials originate in the fact that their conductivity and the band alignment at the interfaces with other materials can be controlled through doping. Here, we consider the ultimate miniaturization of functional devices by computationally investigating the doping of molecular wires suspended between two metal electrodes.[1] For representative systems we find that, upon doping, the molecular conductivity is enhanced by more than two orders of magnitude. We elucidate the microscopic origin of this dramatic effect and present an intuitive picture, which rationalizes our observations in terms of *Fermi-level pinning*. Our results shed new light on recent experimental findings and, most importantly, in-depth understanding of the doping mechanism enables the targeted development of new functional components for sensing and switching at the single-molecule scale.

[1] G. Heimel et al., *Nano Lett.* **9**, 2559 (2009).

CPP 19.4 Tue 10:15 H37

Structure property relationship in aza-bodipy absorber materials for organic photovoltaics — •Roland Gresser, Toni Mueller, Moritz Philipp Hein, Karl Leo, and Moritz Riede — Institute of Applied Photophysics, Dresden University of Technology, Germany

In this joint experimental and theoretical study, we focus on the structure property relationship of aza-bodipy dyes as active donor materials in vacuum deposited small molecule solar cells.

The position of the materials HOMO can be intentionally varied by the choice of the functional group attached to the molecule. The absorption spectra show a red shift of the maximum with increasing donor strength of the substituents due to the increasing HOMO energy and decreasing band gap.

Based on crystal structure data, the charge carrier mobility determining parameters like reorganization energies and transfer integrals are calculated. The results show an increasing molecular orbital overlap and significant higher transfer integrals upon planarization and rigidification of the molecule. With this information, the observed charge carrier mobility differences from experiment can be explained.

In addition to the electronic properties a high thermal and photo stability is essential. From combined thermogravimetric analysis and mass spectroscopy we could determine the degradation process of the material and were able to increase the thermal stability by substitution of the involved species.

CPP 19.5 Tue 10:30 H37

Dicyanovinyl sexithiophenes: self-organization and photovoltaic properties — •Marieta Levichkova[1], David Wynands[1], Alexandr Levin[1], Karl Leo[1], Karsten Walzer[2], Dirk Hildebrandt[2], Peter Bäuerle[3], Rosina Rentenberger[4], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik, TU Dresden, Germany — [2]Heliatek GmbH, Dresden, Germany — [3]Institut für Organische Chemie II und Neue Materialien, Universität Ulm, Germany — [4]Institut für Physik, TU Ilmenau, Germany

Recently, vacuum deposited films consisting of conjugated dicyanovinyl-capped (DCV) oligothiophenes have shown significant potential as photoactive layers in small molecule solar cells [1]. Here, we study the structural and optical properties of films of two DCV-derivatives both comprising six thiophene rings (DCV6Ts) but having different side groups. For both derivatives, neat DCV6T and mixed DCV6T:C60 films are compared using UV-VIS absorption and photoluminescence spectroscopy, X-ray diffraction (XRD), and Atomic Force Microscopy. It is shown that the modification of the molecular structure results in a structured and red shifted absorption band, which indicates better molecular arrangement in the solid state. The improved self-organization at room temperature deposition is confirmed by XRD. Furthermore, the nanomorphology of the mixed DCV6T:C60 films is optimized using substrate heating. Bulk heterojunction solar cells with power conversion efficiencies exceeding 4% are presented.

[1] K. Schulze et al., Adv. Mater. 2006, 18, 2872-2875

15 min. break

CPP 19.6 Tue 11:00 H37

Hexaazatriphenylene and hexaazatrinaphthylene derivatives

as electron transport materials in organic solar cells — •Christiane Falkenberg[1], Martin Baumgarten[2], Ralph Rieger[2], Selina Olthof[1], Karl Leo[1], Moritz Riede[1], and Klaus Müllen[2] — [1]Institut für Angewandte Photophysik, TU Dresden, 01069 Dresden — [2]MPI für Polymerforschung, 55128 Mainz

There is increasing interest in molecularly doped organic materials for the fabrication of efficient organic electronic devices. In small molecule organic solar cells, the so-called p-i-n concept is advantageous for the independent optimization of electrical and optical properties. Here, the absorbing donor-acceptor heterojunction is sandwiched between a p-doped hole transport layer and an n-doped electron transport layer. The design of suitable functional molecules for the transport layers is currently an important issue, however, the choice of available wide-gap materials for the n-side of organic solar cells is very limited. Here, we investigate hexaazatriphenylene and hexaazatrinaphthylene derivatives as substitutes for the common electron transport materials C_{60} or BPhen and BCP. Having bandgaps of > 2.7eV the new materials are transparent which, in combination with a suitable position of the energy levels, enables exciton blocking. Furthermore molecular doping with either acridine orange base (AOB) or NDN1 (Novaled AG) leads to an increase of the conductivity by several orders of magnitude, reaching values beyond $1 \cdot 10^{-6}$ S/cm. Altogether the beneficial optical and electrical properties allow the fabrication of organic solar cells with increased efficiency compared to the standard devices.

CPP 19.7 Tue 11:15 H37

Structure - property relationship of thiophene based materials bearing different accepting groups — •Marion Wrackmeyer, Markus Hummert, Horst Hartmann, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, Technische Universität Dresden, Germany

Organic solar cells require new materials for improved efficiencies. The relationship of molecular structure and properties is very important to optimise the devices. An interesting class of materials are thiophene block co-oligomers. The materials obtain electron donating (D) and accepting (A) groups and have the general structure A-D-A or D-A-D. In particular, the investigation of electron accepting groups is very important, because they have a high influence on the electronic structure of an organic molecule and are therefore an influential impact in the performance of a small molecule p-i-n solar cell. We present investigations on thiophene based materials bearing different accepting groups. The accepting groups are eg dicyanovinyl, dioxaborine, and benzthiadiazole. The materials were synthesised by Stille-coupling. Basic precondition for all materials is the thermal stability for deposition by vacuum-techniques. Subsequent investigations focus on absorption (solution and thin films), electrochemical behaviour (cyclic voltammetry to investigate the frontier molecular orbital energy levels), DFT-calculations (to show the location of HOMO and LUMO), mobility, morphology, dopability, and the properties of a solar cell.

CPP 19.8 Tue 11:30 H37

Charge transport in self-assembled semiconducting organic layers: role of dynamic and static disorder — •Thorsten Vehoff[1], Yeon Sook Chung[2], Karen Johnston[1], Alessandro Troisi[3], Do Yeung Yoon[2], and Denis Andrienko[1] — [1]Max Planck Institut fuer Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany — [2]Department of Chemistry, Seoul National University, Seoul 151-747, Republic of Korea — [3]Department of Chemistry and Centre of Scientific Computing, University of Warwick, Coventry, CV4 7AL, United Kingdom

Partial disorder is an inherent property of self-assembled organic semiconductors that complicates their rational design, since electronic structure, self-assembling properties and stability all have to be accounted for simultaneously. Therefore, the understanding of charge transport mechanisms in these systems is still in its infancy. A theoretical study of charge transport in organic semiconductors was performed on self-assembled layers of [1]Benzothieno[3,2-b]benzothiophene functionalized with alkyl side chains. Analysis showed that semiclassical dynamics misses static (on timescales of charge transport) disorder while the solution of the master equation combined with the high-temperature limit Marcus theory for charge transfer rates does not take into account molecular dynamic modes relaxing on a timescale of charge hopping. A comparison between predictions based on a perfectly ordered and a realistic crystal structure reveals the strong influence of static and dynamic disorder. The advantage of two-dimensional charge transporting materials over one-dimensional ones is clearly shown.

CPP 19.9 Tue 11:45 H37

Charge Transport in rr-P3HT:PCBM Blends - The Impact of Ultrahigh Regioregularity on Hole Transport and Device Performance — •Ralf Mauer and Frédéric Laquai — Max-Planck-Institut für Polymerforschung, Mainz, Deutschland

Blends of poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl C_{61} butyric acid methyl ester (PCBM) have emerged as a prototypical material system for bulk heterojunction solar cells with reasonable efficiencies during the past five years. Despite tremendous engineering efforts to push devices to 5% power conversion efficiency (PCE), the correlation between charge carrier mobility and device performance is still up for debate. Theoretical models range from "the higher - the better" over optimum finite mobilities to no effect of mobility on PCE at all.

We investigate charge transport in pristine P3HT films and in blends with PCBM by the time of flight (TOF) technique and analyse the results in the framework of the Gaussian disorder model. In order to understand the effect of charge transport on solar cell efficiency, we examine P3HT with three different regioregularities, i.e. regiorandom P3HT, rr-P3HT with high (rr=94%) and with ultrahigh (rr>98%) regioregularity. While the regioregularity is known to have a strong influence on the charge carrier mobility, its effect on other transport parameters, especially on the energetic disorder of hole transport in P3HT, is reported by us for the first time.

Finally, we correlate the TOF results and spectroscopic measurements with device performance to determine the influence of charge transport on the power conversion efficiency.

CPP 19.10 Tue 12:00 H37

Charge transport in conjugated polymers with energetic disorder — •James C Blakesley[1,2], Helen S Clubb[1], Christopher Groves[1], Louise M Hopkins[1], and Neil C Greenham[1] — [1]University of Cambridge, Cambridge, UK — [2]Universität Potsdam, Potsdam, Germany

We investigate charge transport in sandwich-type devices with two polyfluorene-based copolymers: poly(9,9-dioctylfluorene-co-bis(N,N'-(4,butylphenyl))bis(N,N'-phenyl-1,4-phenylene)diamine) (PFB) and poly(9,9-dioctylfluorene-co-benzothiadiazole) (F8BT). A standard analysis of the data produces a poor fit to the data, with an apparent dependence of mobility on device thickness. Previously, such behaviour in electron transport has been attributed to trapping[1]. However, we find that a good fit is obtained by using a numerical simulation based on energetic disorder that takes into account the effects of electric field and carrier density on mobility (Extended Gaussian Disorder model). The amount of energetic disorder is quantified by 110+/-10meV and 100+/-10meV respectively. When the two materials are blended together, hole mobility remains constant when the fraction of PFB is 50% or greater, but drops dramatically for low concentrations of PFB. The amount of energetic disorder remains unaffected by any degree of blending, suggesting that there is no change in microscopic ordering of the polymers upon blending.

[1] R. Steyrleuthner, S. Bange and D. Neher, J. Appl. Phys. 105, 064509 (2009)

CPP 19.11 Tue 12:15 H37

Towards high charge carrier mobilities by rational design of organic semiconductors — •Denis Andrienko[1], Valentina Marcon[2], James Kirkpatrick[3], Victor Ruehle[1], Bjoern Baumeier[1], Thorsten Vehoff[1], Alexander Lukyanov[1], Kurt Kremer[1], Jenny Nelson[3], and Christian Lennartz[4] — [1]Max Planck Institute for Polymer Research, Mainz — [2]Technische Universität Darmstadt, Germany — [3]Imperial College London, UK — [4]BASF AG, Ludwigshafen

The role of material morphology on charge carrier mobility in partially disordered organic semiconductors is discussed for several classes of materials: derivatives of hexabenzocoronenens [1], perylenediimides [2], triangularly-shaped polyaromatic hydrocarbons [3], and Alq3. Simulations are performed using a package developed by Imperial College, London and Max Planck Institute for Polymer Research, Mainz (votca.org). This package combines several techniques into one scheme: quantum chemical methods for the calculation of molecular electronic structures and reorganization energies; molecular dynamics and systematic coarse-graining approaches for simulation of self-assembly and relative positions and orientations of molecules on large scales; kinetic Monte Carlo and master equation for studies of charge transport.

[1] J. Kirkpatrick, et al, Phys. Rev. Lett., 98, 227402, 2007; [2] V. Marcon, et al, J. Am. Chem. Soc., 131, 11426, 2009; [3] X. Feng et al,

Nature Materials 8, 421, 2009

CPP 19.12 Tue 12:30 H37

Fully functionalized block copolymers for organic electronic applications — •Sven Hüttner[1,2], Michael Sommer[2], Justin Hodgkiss[1], Peter Kohn[3], Thomas Thurn-Albrecht[3], Richard Friend[1], Ullrich Steiner[1], and Mukundan Thelakkat[2] — [1]Cavendish Laboratory, University of Cambridge — [2]Angewandte Funktionspolymere, Makromolekulare Chemie I, Universität Bayreuth — [3]Experimentelle Polymerphysik, Universität Halle-Wittenberg

Block copolymers are well known to phase separate in highly ordered nanostructures on length scales commensurate with the exciton diffusion length. We use fully functionalized block copolymers for photovoltaic devices, where a donor and an acceptor polymer are covalently linked. The acceptor block consists of a polyacrylate backbone with pendant perylene bisimide moieties and the donor block consists of poly(3-hexylthiophene) (P3HT). We combine temperature dependent small angle and wide-angle X-ray scattering measurements to investigate the block copolymer phase separation as well as the influence of the crystallisation kinetics of the two blocks. Intermolecular and intramolecular interactions drive the self-assembly of structures from molecular lengthscales to larger mesostructures of some nanometers to microphase separation of some tens of nanometers. The investigation of the morphology is accompanied by steady state spectroscopy and transient absorption spectroscopy. Furthermore organic thin film transistors are used to characterize the transport properties in these novel materials which are found to exhibit unique properties such as the tunability between n-type, p-type or ambipolar transport.

CPP 20: Organic Electronics and Photovoltaics II

Time: Tuesday 13:45–16:15 Location: H37

CPP 20.1 Tue 13:45 H37

Spectroscopic signatures of C_{70}-Anions in Polymer-Fullerene composites — •Andreas Sperlich[1], Moritz Liedtke[2], Hannes Kraus[1], Oleg Poluektov[4], Carsten Deibel[1], Nazario Martin[3], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, Div. Functional Materials for Energy Technology, D-97074 Würzburg — [3]Departamento de Quimica Organica, Facultad de Quimica, Universidad Complutense, E-28040 Madrid — [4]Chemical Sciences and Engineering Division, Argonne National Laboratory, 9700, USA

C_{70}-derivates are used in the most efficient organic bulk heterojunction solar cells. However, the detailed photophysical processes in composites containing C_{70} are still unresolved. In this contribution, our focus is on the light-induced charge transfer from the polymer to the fullerene, generating negatively charged C_{70} radicals. Photoinduced absorption (PIA), electron spin resonance (ESR 9.5GHz) and optically detected magnetic resonance (ODMR) were used to draw a picture of the photoinduced charge transfer from polymers to C_{70}. We provide the first experimental identification of the light induced C_{70} radical anion in blends with P3HT using high frequency ESR (130GHz). Comparing spectra from C_{70}-derivates with different sidechains, we could confirm that the electron is indeed localized on the C_{70}-cage. Further, we identify an additional absorption band at 0.9eV due to C_{70}^{-} by PIA.

CPP 20.2 Tue 14:00 H37

The Localized Nature of Charge Transfer in F_4TCNQ-Doped Thiophene-Based Donor Polymers — •Patrick Pingel[1], Lingyun Zhu[2], Kue Surk Park[1], Jörn-Oliver Vogel[1], Silvia Janietz[3], Eung-Gun Kim[2], Jürgen P. Rabe[1], Jean-Luc Brédas[2], and Norbert Koch[1] — [1]Department of Physics, Humboldt University Berlin, Germany — [2]School of Chemistry and Biochemistry, and Center for Organic Photonics and Electronics, Georgia Institute of Technology, USA — [3]Fraunhofer IAP, Potsdam, Germany

Recently, polymer layers exhibited exceptionally high conductivities upon p-type doping with the molecular acceptor tetrafluorotetracyanoquinodimethane (F_4TCNQ). Here, we present experimental and theoretical results on blend layers of F_4TCNQ and a series of poly(3-hexylthiophene-*co*-dithienyltetrafluorobenzene) (P3HT-TFT) copolymers with systematically varied TFT content. Regardless of the amount of TFT in the donor polymer, we find that only a single charge transfer (CT) species is formed, which we assign to the interaction of F_4TCNQ with an oligothiophene segment of the main chain. The degree of CT remains constant, even if the dopant concentration is increased up to a point, where closely neighbouring CT complexes exist at the same uninterrupted thiophene segment. Our findings show that the CT between F_4TCNQ and an oligothiophene segment has a localized, isolated nature, possibly comprising less than five connected thiophene units. Thus, CT is dictated by the local electronic structure on the nm scale, rather than depending, e.g., on the macroscopic ionization potential determined from photoemission methods.

CPP 20.3 Tue 14:15 H37

Charge Transfer Exciton Dynamics in Polymer/Fullerene Blend — •Josef M. Berger, Markus Hallermann, Enrico Da Como, and Jochen Feldmann — Lehrstuhl für Photonik und Optoelektronik, CeNS, LMU München

Polymer fullerene blends are one of the most promising material systems for organic photovoltaics. A major loss channel in these cells is the formation and recombination of charge transfer excitons. These excitons emit light as a consequence of radiative recombination of the hole on the polymer and the electron on the fullerene [1]. Here, we report on time resolved emission experiments with the aim of understanding the parameters controlling the recombination lifetime. For the blend of MDMO-PPV/PCBM we correlate the decay profile with the morphology obtained by transmission electron microscopy [2]. [1] Markus Hallermann, Stephan Haneder, and Enrico Da Como, Appl. Phys. Lett 93, 053307 (2008) [2] Markus Hallermann, Ilka Kriegel, Enrico Da Como, Josef M. Berger, Elizabeth von Hauff, Jochen Feldmann, Advanced Functional Materials 19, 3662 (2009)

CPP 20.4 Tue 14:30 H37

The Relationship between the Electric Field Induced Dissociation of Charge Transfer (CT) Excitons and the Photocurrent in Novel Hybrid Small Molecular/Polymeric Solar Cells — •Sahika Inal[1], Alan Sellinger[2], and Dieter Neher[1] — [1]Universität Potsdam, Institut für Physik und Astronomie, 14476 Potsdam-Golm — [2]Institute of Materials Research & Engineering, Singapore 117602

Complete dissociation of coulombically bound interfacial states is an ultimate step accounting for photovoltaic performance. Recent work has proposed that the emission of CT-exciton, i.e. an exciplex, is a competing process to the generation of free charges [Appl. Phys. Lett. 2007, 90, 092117]. Here, we investigated the photophysical processes in a bulk heterojunction system using a soluble poly(p-phenylenevinylene) donor and a novel small molecular electron acceptor based on Vinazene (2-vinyl-4,5-dicyanoimidazole). Recent work has shown that this blend exhibits a featureless emission, prominent at long wavelengths of the spectrum, which was attributed to a CT-exciton [J. Chem. Phys. 2009, 130, 094703]. We monitored the field induced dissociation of these CT-excitons by means of steady state and time resolved PL spectroscopy. Shortened decay times and reduced PL emission in blend film evidence the dissociation of the emissive intermolecular pair by the external electric field. Analyzing the dependence of the photocurrent and external quantum efficiency on the external field, the fate of the separated exciplex pairs is tackled. It is suggested that the formation of free carriers involves channels other than CT-excitons in such blends.

CPP 20.5 Tue 14:45 H37

Study of Sub-Bandgap States in Polymer-Fullerene Solar Cells — •Martin Presselt[1], Felix Herrmann[1], Marco Seeland[1], Maik Bärenklau[1], Sebastian Engmann[1], Roland Rösch[1], Wichard J. D. Beenken[2], Sviatoslav Shokhovets[1], Harald Hoppe[1], and Gerhard Gobsch[1] — [1]Experimental Physics I, Institute of Physics & Institute of Micro- und Nanotechnologies, Ilmenau University of Technology, Weimarer Str. 32, 98693 Ilmenau, Germany — [2]Theoretical Physics I, Institute of Physics, Ilmenau University of Technology, Weimarer Str. 25, 98693 Ilmenau, Germany

At present polymer-fullerene blends are widely used to build organic solar cells. The main contribution to their photocurrent originates from optical transitions between occupied states below the HOMO level and unoccupied states above the LUMO level of the polymer.

In this work, we investigated the origin of states contributing to the optical absorption in the sub-bandgap spectral range and the resulting photocurrent in P3HT-PCBM bulk heterojunction solar cells. Photothermal deflection spectroscopy, temperature dependent external quantum efficiency, photoluminescence and electroluminescence as well as spectroscopic ellipsometry measurements have been carried out. Effects due to different P3HT-PCBM blending ratios and annealing temperatures have been studied.

Two models are discussed to explain the experimental observations: optical transitions involving (a) disorder and/or defect related states, and (b) charge transfer complexes.

CPP 20.6 Tue 15:00 H37

Influence of system size on simulated charge mobility in amorphous films of tris(8-hydroxyquinolinato)aluminium (Alq3) — •Alexander Lukyanov and Denis Andrienko — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

We present the results of a modeling study of the charge transport in amorphous films of tris(8-hydroxyquinolinato)aluminium (Alq3). In our multiscale approach we combine molecular dynamics to generate material morphologies, Marcus theory to evaluate charge hopping rates and kinetic Monte Carlo to simulate charge dynamics. Energetic disorder is taken into account by assigning partial charges to the hopping sites, obtained from DFT B3LYP, 6-311g(d) calculations. In contrast to the previous studies Poole-Frenkel behavior of the mobility is reproduced. Our results indicate strong finite-size effects, meaning that the absolute value of the calculated mobility decreases with the increase of the simulation box size. Simple analogy with a classical percolation problem suggests that very large systems are required to obtain a reliable estimate of the charge carrier mobility.

CPP 20.7 Tue 15:15 H37

Influence of injection and extraction barriers realized by choice of donor and HTL on organic solar cell performance — •Wolfgang Tress, Ellen Siebert, Karl Leo, and Moritz Riede — TU Dresden, Institut für Angewandte Photophysik

In the p-i-n solar cell architecture, the active materials of a donor/acceptor flat heterojunction are sandwiched between two doped transport layers, which provide a highly conductive contact to the cathode metal and the ITO, respectively. This concept allows for a systematic study of the influence of the HOMO of the donor and the adjacent hole transport layer (HTL) on the open circuit voltage (V_{oc}) and the shape of the IV curve. This approach avoids the main problems emerging by metal-organic interfaces like varying work functions, unpredictable interface dipoles, etc.. Additionally, extraction barriers, which cannot be realized by the choice of metal, can be adjusted in a controlled way by a HOMO of the HTL lying deeper than the HOMO of the donor. Using donor and HTL materials with a HOMO between 5.0 and 5.6 eV in combination with C_{60} as acceptor, we demonstrate a systematic dependence of V_{oc} on the HOMO of the donor, whereas the built in field is goverened by the HOMO of the strongly doped HTL. The fill factor (FF) is mainly influenced by the HOMO offset between donor and HTL. Both types of barriers (extraction and injection) decrease FF resulting in s-shaped curves with different characteristics. The experimental results are interpreted by comparison to simulation data of a drift-diffusion model, treating the HOMO barrier with a field dependent lowering effect.

CPP 20.8 Tue 15:30 H37

Hole transport characteristics of pentacene studied with Green functions and real-time propagation — •Sebastian Radke[1], Caroline Gollub[1,2], Stanislav Avdoshenko[1], Rafael Gutiérrez[1], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology — [2]Max Planck Institute for the Physics of complex Systems, Dresden

For temperatures higher than 150 Kelvin the charge carrier mobility in organic semiconductors depends sensitively upon an interplay of bandlike and hopping transport [1]. In this contribution, the hole transport characteristics of an organic semiconducting material are studied with two different theoretical methods and both approaches are compared. As a model system a pentacene structure is selected, which is well-characterized in the context of organic electronics. The first approach is based on a Green function formulation of the Holstein-Peierls model, accounting for local and non-local electron-phonon coupling and it addresses the transport problem in the energy space, so that fluctuations are taken into account only within a static picture. In the second approach, a real-time propagation of the charge carrier wave function is performed and this provides a deeper insight into the different time scales appearing in the problem. The Hamiltonian is formulated in the tight-binding representation, where the parametrization is evaluated for different levels of theory of the MD trajectories and of the electronic structure calculations.

[1] Y. C. Cheng, *et al.*, J. Chem. Phys. **118**, 3764 (2002).

CPP 20.9 Tue 15:45 H37

Ab initio based modeling of charge transport in organic semiconductors — •Caroline Gollub[1,2], Stanislav Avdoshenko[1], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology — [2]Max Planck Institute for the Physics of complex Systems, Dresden

In organic electronics, theory is expected to play an important role for the search of organic semiconducting materials with improved charge carrier mobilities. Current theoretical efforts are devoted to the understanding of the charge transport mechanism and the accurate prediction of the structure-mobility relationship. In this contribution, an approach for the charge migration in organic semicondutors is presented based on a self-consistent propagation of the charge carrier wave function effected by the molecular dynamics of the system, i.e. the electronic and nuclear dynamics are treated on an equal footing. The simulation comprises the evaluation of charge transfer parameters from ab initio calculations, the quantum dynamical calculation of the evolution of the charge carrier wave function and the molecular dynamics of the studied system. The method allows to follow the real-time and real-space transport and can be used to extract charge carrier mobilities in dependence of the chemical functionality, the temperature or the structure assembly. The technique will be demonstrated for hole transport in a 1D stack of coronene molecules.

CPP 20.10 Tue 16:00 H37

Energetics of Excited States in the Conjugated Polymer Poly(3-hexylthiophene) — Julien Gorenflot[1], •Daniel Mack[1], Daniel Rauh[4], Stefan Krause[2], Carsten Deibel[1], Achim Schöll[2], Friedrich Reinert[2,3], and Vladimir Dyakonov[1,4] — [1]Experimental Physics VI, University of Würzburg, D-97074 Würzburg — [2]Experimental Physics II, University of Würzburg, D-97074 Würzburg — [3]FZK Karlsruhe, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe — [4]Bavarian Centre for Applied Energy Research (ZAE Bayern), D-97074 Würzburg

Although prototypes and first commercial polymer-based solar panels already exist, a comprehensive understanding of the fundamental processes and energetics involved in photocurrent generation is still missing and limits further device optimisations. We present a complementary set of experiments on poly(3-hexylthiophene(P3HT), which enables us to draw general conclusions on the energy levels and barriers involved in the processes from light absorption to polaron pair dissociation. From photoemission spectroscopy of occupied and unoccupied states we determine the transport gap to 2.6 eV, which we show to be in agreement with the onset of photoconductivity by spectrally resolved photocurrent measurements. We also find that photogenerated singlet excitons, generated with light at the absorption edge, require 0.7 eV of excess energy to overcome the binding energy. The intermediate charge transfer state, also called polaron pair, is situated only 0.3 eV above the singlet exciton. We discuss our results in view of their impact on charge generation.

CPP 21: Organic Electronics and Photovoltaics III

Time: Wednesday 9:30–12:45 Location: H37

CPP 21.1 Wed 9:30 H37

High-resolution spectroscopic mapping of P3HT:PCBM organic blend films for solar-cell applications — •Xiao Wang[1], Dai Zhang[1], Kai Braun[1], Hans-Joachim Egelhaaf[2], Christoph J. Brabec[2], and Alfred J. Meixner[1] — [1]Institute of Physical and Theoretical Chemistry, University of Tübingen — [2]Konarka Technologies GmbH, Nürnberg

We present a high resolution near-field spectroscopic mapping of the poly(3-hexylthiophene) and [6, 6]-penyl-C61 butyric acid methyl ester (P3HT:PCBM) blend film upon different thermal annealing.[1] From the simultaneously recorded morphology and spectroscopic information, the interplay among the blend film morphology, the local P3HT:PCBM molecular distribution, and the P3HT photoluminescence (PL) quenching efficiency were discussed. The PL and Raman signals of the electron donor (P3HT) and acceptor (PCBM) have been probed at an optical resolution of approximately 10 nm which allow the direct identification of the chemical nature of the different domains. Moreover, we were able to reveal and quantify local quenching, which is related to the electron transfer from P3HT to PCBM. Based on the experimental results, it is proposed that high resolution near-field spectroscopic imaging proves its clear capability of mapping the local chemical composition and photophysics of the P3HT:PCBM blends on a length of a few nanometers.

[1] X. Wang, et al. Advanced Functional Materials (in press)

CPP 21.2 Wed 9:45 H37

Investigations on thickness dependence of electrical characteristics and stability of self-assembled monolayers — •Dana Habich — FAU Erlangen-Nürnberg, Institute of Polymer Materials

We investigated the influence of the molecular chain length (n) of aliphatic Cn-phosphonic acids on the electrical characteristics of self-assembled monolayers (SAMs) based on these molecules. SAMs prepared on aluminium/aluminium oxide (Al/AlOx) and conductive indium tin oxide (ITO) substrates behave as molecular dielectric layer. In integrated devices (e.g. capacitors) with activated Al-bottom electrode, the dielectric layer is created from a double-layer AlOx/SAM. Capacitance and breakdown voltage correlates monotonically with the SAM thickness, the current density at low voltage does not follow the expected correlations in detail. We address this behavior to morphological changes of the SAMs on AlOx, from an amorphous structure for short chains to a crystalline state for longer alkyl chains. To decouple the relative contributions of the AlOx and the SAM to the insulation, an independent analytical approach to characterize the SAM was chosen: cyclic voltammetry on SAM decorated ITO. The faradic current of a redox active compound in solution is indirect proportional to the molecular chain length. Qualitatively, this observation proofs the conclusions from the capacitor measurements. The system ITO/SAM, further provide an approach for functional coatings on ITO with the possibility to tune addressability and stability of the electrodes. Stability was investigated by static contact angle and STM measurements before and after electrical stress. Ref.: Org. Electron. 10 (2009) 1442.

CPP 21.3 Wed 10:00 H37

2D mapping of the Electron Beam Induced Current (EBIC) in organic solar cells — •Piet Reuter[1], Thomas Rath[2], Gregor Trimmel[2], and Peter Hadley[1] — [1]Institute of Solid State Physics, TU Graz, A-8010 Graz, Austria — [2]Institute for Chemistry and Technology of Materials & Christian Doppler Laboratory for Nanocomposite Solar Cells, TU Graz, A-8010 Graz, Austria

Electron Beam Induced Current (EBIC) measurements were used to produce 2D nanoscale maps for investigating the homogeneity of solar cells. These maps are acquired by putting the electron beam of a scanning electron microscope (SEM) in spot mode and using a programmable sample stage to move the solar cell under the stationary beam. The electron beam generates electron-hole pairs in the solar cell much like light does in normal operation. The variations in the EBIC signal can be attributed to changes in the morphology. By comparing these measurements with morphological information of the devices, one can identify the cause of inferior performance which should then lead to an improvement of further devices. It should be mentioned that long time exposures to an electron beam destroys the organic semiconductors. Studies were performed to determine the acceptable electron dose during the measurement.

CPP 21.4 Wed 10:15 H37

Analysis of Metallic Conduction at the Interface of TTF and TCNQ Crystals. — •Viktor Atalla, Mina Yoon, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, Germany

Organic materials are promising candidates for a next generation of electronic devices, since they offer a variety of new intriguing electronic phenomena while being environmentally friendly, low cost, and mechanically flexible. Here we study the interface of tetrathiofulvalene (TTF) and 7,7,8,8-tetracyanoquinodimethane (TCNQ) organic molecular crystals which was found to exhibit metallic conduction [1] whereas the individual crystals are large band-gap semiconductors. Using quantum mechanical first-principles approaches employing the FHI-aims code [2] basic properties of monomers, dimers, and individual crystals are investigated. We construct interfaces between the two types of crystals and study the electronic band structures of the interface-induced states, which are relevant to the charge transport properties of the material. Depending on the relative orientation of the crystals the band structures were found to indicate metallic conduction at the interface. Furthermore the energetics of the polaron is investigated by calculating the geometry relaxation energy. For monomers of TTF and TCNQ this is found to be in the order of 0.1 eV, indicating that the electron-lattice interaction is an important parameter for charge transport in this system. [1] H. Alves et al., Nat. Mat. 7, 574 (2008). [2] V. Blum et al., Comp. Phys. Comm. 180, 2175 (2009).

CPP 21.5 Wed 10:30 H37

Structural analysis of photoactive polymer blend films on textured polymeric and inorganic substrates — •Robert Meier[1], Matthias A. Ruderer[1], Gunar Kaune[1], Alexander Diethert[1], Fabian Markl[1], Volker Körstgens[1], Johannes Wiedersich[1], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department LS E13, James-Franck-Straße 1, 85747 Garching — [2]HASYLAB at DESY, Notkestraße 85, 22603 Hamburg

Due to their large chemical variety photoactive conducting polymers are of great interest for versatile applications such as organic photovoltaics. In order to improve the device characteristics not only the polymer film but also the rest of the device has to be optimized regarding light absorption and charge carrier separation. Therefore the focus of this work is put on the use of structured substrates in order to improve the light absorption and the overall device performance. A new route based on solution casting is introduced to structure the electron blocking PEDOT:PSS layer. Absorption spectra of polymer blend films spincoated on such structured substrates show promising aspects for their suitability for organic photovolatics. In addition the inner film morphology of a polymer blend based on M3EH-PPV and F8BT spincoated on structured channel-like substrates is investigated using GISAXS measurements. The obtained results show a dependence of the film morphology and the topographic shape on the etched depth of the channels. The study is complemented with atomic force and scanning electron microscopy measurements.

15 min. break

CPP 21.6 Wed 11:00 H37

Structural and morphological changes in P3HT thin film transistors applying an electric field — •Deepak kumar Tiwari[1], Souren Grigorian[1], Ullrich Pietsch[1], Heinz Flesch[1,2], and Roland Resel[1,2] — [1]University of siegen, siegen, Germany — [2]Graz University of technology

We report on electric field dependent crystalline structure and morphological changes of drop casting and spin coated poly(3-hexyltheiopine) (P3HT) thin films. In order to probe the morphological changes induced by an applied electric field the samples were covered with thin source/drain electrodes separated by a small channel of 2 mm width. A series of x-ray reflectivity, X-ray grazing incidence out-of-plane and in-plane scans have been performed as function of the applied electric voltage. The (100) peak shows a decrease in intensity with increase of the applied electric field. This might be caused by Joule heating and the creation of current induced defects in the P3HT film. On other hand the (020) peak intensity shows much stronger changes with applied field. Considering the *-* stacking direction the measured effect can be directly related to a change in the electric transport. The observed changes in structure are reversible and the current-voltage cycle can be repeated several times. For X-ray reflectivity major changes have been found close to critical angle of total external reflection indicating the film becomes less dense and increases in surface roughness with increase of the voltage. This change in surface behaviour could be confirmed by in-situ AFM measurements.

CPP 21.7 Wed 11:15 H37

Thickness dependent structural order in P3HT films - a key parameter for high OFET mobility — •Benedikt Gburek, Richa Sharma, Torsten Balster, and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Applications of organic electronics require cheap and fast production methods on flexible substrates. Following these goals, top-gate OFETs on PET foils were used to analyze the dependence of the device characteristics on the crucial parameter of semiconductor layer thickness. The organic semiconductor, regio-regular P3HT, and the gate insulator were deposited by spin-coating under atmospheric conditions.

The charge carrier mobility was found to be rather low for extremely thin layers of several nanometers only. However, with increasing layer thickness, mobility increases by two orders of magnitude until a "saturation thickness" of 50 nm, above which it remains constant.

Further details of the ordering were extracted according to the Vissenberg-Matters model with gate-voltage dependent mobility $\mu = \mu_0 \left(\left(V_{GS} - V_{th} \right) / 1V \right)^{\gamma}$, where γ is directly related to the width of the density of states. The analysis reveals that the disorder parameter γ decreases from 3.1 to 1.0 over the examined thickness range, which explains the low mobility of thinner films by higher energetic disorder.

This analysis proves to be highly advantageous as it represents the whole transfer curve, gives better comparability and offers more physical insight. Our study demonstrates the crucial role of layer thickness tuning for improved film structure and optimum material performance.

CPP 21.8 Wed 11:30 H37

Deposition of P3HT via dip coating onto transistors with channel lengths below 1 μm — •Silviu Botnarash, Steve Pittner, and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, D-28759, Germany

A high quality interface between the organic semiconductor and the oxide is crucial for the high performance of an OFET. A good surface treatment is imperative, but it will lower the surface energy of the oxide, making it difficult to spin coat on it uniform semiconductor layers from solvents like chloroform or toluene. We report on the usage of the dip coating technique to achieve highly ordered layers of regioregular poly(3-hexylthiophene) (rr-P3HT). By varying the removal speed of the silicon substrate from solution, the concentration of the solution or both, one can achieve ultrathin layers of rr-P3HT which permit to analyze OFET properties in the sub-monolayer regime. Decreasing the channel length of the transistors down to the range of the contour length of the rr-P3HT is expected to improve the characteristics of the OFET's. An additionally applied electric field between the source and drain electrodes during dip coating facilitates the trapping of P3HT molecules on the electrodes increasing the performance of the device. We used rr-P3HT with an average contour length of 80-100 nm. Compared to previously reported results for chloroform based solutions, the same concentration range of rr-P3HT in toluene displayed better characteristics, which is believed to be due to lower evaporation rate of toluene. Subsequent drying in a nitrogen rich atmosphere over a period of up to 24 h positively influences the performance of the OFET's.

CPP 21.9 Wed 11:45 H37

Semitransparent small-molecule organic solar cells — •Jan Meiss[1], Christian Uhrich[2], Stefan Sonntag[2], Wolf-Michael Gnehr[2], Martin Pfeiffer[2], Karl Leo[1], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]heliatek GmbH, Liebigstraße 26, 01187 Dresden, Germany

Semitransparent, colourful solar cells are of interest for a wide range of applications, e.g. sun shading of residential and office buildings or cars. Previously, among organics-containing devices, only semitransparent dye-sensitized solar cells showed power conversion efficiencies (PCE) that allowed first meaningful applications, whereas semi-transparent small-molecule organic solar cells (OSC) were limited to PCE well below 1%.

We present small-molecule semitransparent OSC deposited by thermal vacuum evaporation on ITO-coated glass. The organic materials include absorber materials and doped dedicated charge transport layers. Due to our unique device architecture, the top electrode is ITO-free, consisting only of an ultra-thin multi-layer metal film.

The OSC exhibit light transmission in the visible range of 30-50% with PCE of over 2%. Organic capping layers are used to significantly lower reflection and increase transmission without significant loss of PCE. Furthermore, we have achieved first large-area semitransparent tandem OSC with 3.5% PCE at 20-40% transmission in the visible range on 4cm^2, which show the potential of this type of device for large-scale building integration.

CPP 21.10 Wed 12:00 H37

Stability optimisation of small molecule organic solar cells — •Martin Hermenau, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, George-Bähr-Str. 1, 01069 Dresden

In addition to high efficiency and low cost, a long device lifetime is a crucially important factor for the commercialisation of small molecule organic solar cells. Previous results mostly covered unencapsulated devices and showed low lifetimes under 1000 hours even without permanent illumination.

Here, we present results on improving the intrinsic stability of glass-glass-encapsulated p-i-n solar cells containing small molecules. Zinc-Phthalocyanine and the fullerene C$_{60}$ are used as photoactive materials. Doped layers of wide gap materials and C$_{60}$ are used as hole and electron transport layer, respectively. All devices are illuminated with monochromatic or white LEDs and IV characteristics are automatically recorded during the entire measuring period.

In contrast to polymer solar cells, we do not observe an influence of different types of top contact materials on the lifetime. All variations of Gold, Silver and Aluminium lead to stable cells for about 1500 hours of continued illumination.

However, by changing the type and even the thickness of the hole transport material we are able to enhance the extrapolated lifetime (t80) from about 1100 hours with 30nm PV-TPD up to more than 5000 hours with 60nm Di-NPB. These results are achieved with encapsulated devices and illumination intensitites up to 840 mW/cm^2 from high-power white LEDs at controlled temperatures of 50°C.

CPP 21.11 Wed 12:15 H37

Self organized molecular electronic junctions using two phase liquid structures in microfluidic channels — •Shashi Thutupalli[1], Mark Elbing[2], Matthias Fischer[2], David Muñoz[3], Ralf Seemann[1,4], Marcel Mayor[2,3], and Stephan Herminghaus[1] — [1]MPI for Dynamics and Self Organization, Göttingen, Germany — [2]Forschungszentrum Karlsruhe GmbH, Institute for Nanotechnology, Karlsruhe, Germany — [3]University of Basel, Department of Chemistry, Basel, Switzerland — [4]Experimental Physics, Saarland University, Saarbrücken, Germany

Using a combination of microfluidics and molecular design, we demonstrate self assembled, reconfigurable molecular electronic junctions. To construct metal-molecule-metal junctions, we employ liquid mercury as the electrode contact in crossed microfluidic channels. Self assembled monolayers (SAM's) of conducting molecular rods are created on the surface of the mercury, which are then bridged to the other mercury electrode via microfluidic control. By precise flow control, we create rectifying molecular junctions using asymmetric molecules. We report on the electrical properties of these microfluidic metal-molecule-metal junctions. Also, we use surfactant stabilized foam-like water-in-oil emulsions to form variable molecular junctions. Here, molecules synthesized with hydrophobic conducting cores and hydrophilic ends self-insert into the lamellae between aqueous droplets. Using the aqueous droplets then as the molecular contacts, we report on the conducting properties of the inserted molecules and demonstrate the possibility of reconfigurable circuits using topological droplet rearrangements.

CPP 21.12 Wed 12:30 H37

DNA Based Molecular Electronics Using Mercury Droplets in Microfluidic Channels — •Shuang Hou, Shashi Thutupalli, and Stephan Herminghaus — Max Planck Institute for Dynamics and Self Organization, D-37073, Göttingen, Germany

Mercury droplets in microfluidic channels are used as electrodes to investigate the electronic properties of single strand DNA (ssDNA) molecules. In this system, a self assembled monolayer (SAM) of thiolated DNA oligomers (˜ 5 nm length) of specific base sequences is formed on the surface of mercury droplets. Two such droplets are then brought together by microfluidic manipulation to form a mercury-ssDNA-mercury electrical junction. We identified single SAMs of ssDNA oligos, double SAMs of ssDNA oligos of the same composition, and complementary binding DNA composed junctions. Here, we report the influence of base pair type and DNA sequence length to the electronic characteristics. On the basis of these results, the design of DNA based molecular electronic elements (such as diodes) seems possible.

CPP 22: Biopolymers and Biomaterials (jointly with BP)

Time: Wednesday 14:00–17:30 Location: H37

Topical Talk CPP 22.1 Wed 14:00 H37

Atomic Layer Deposition (ALD) as a Versatile Tool for Nanoscience — •Mato Knez[1], Seung-Mo Lee[1], Adriana Szeghalmi[1], Yong Qin[1], Eckhard Pippel[1], Christian Dresbach[2], and Gerd Hause[3] — [1]Max-Planck-Institute of Microstructure Physics, Halle, Germany — [2]Fraunhofer Institute IWM, Halle, Germany — [3]Martin-Luther-University, Halle-Wittenberg, Germany

Atomic layer deposition (ALD) is a thin film deposition technique which was developed in the 1970s to meet the needs for processing thin film electroluminescent displays (TFEL). Being a non-line-of-sight deposition technique, ALD allows for good coating conformality even with 3D nanostructured substrates or structures with a high aspect ratio together with a good capability for upscaling. An increasing number of researchers make use of the precision of ALD for fabrication or functionalization of nanostructures, optical coatings, catalytically active coatings, encapsulation, corrosion protection or even infiltration of soft materials with metals.

The most recently evolving application of ALD deals with the modification of mechanical properties of soft materials after infiltration of metals by ALD. Although the detailed chemistry behind the approach is not yet understood, biological materials, such as spider silk or collagen, can positively change their mechanical properties after being treated with pulsed vapors of metal precursors. The toughness of such materials increased by up to 10-fold, outperforming most manmade materials.

CPP 22.2 Wed 14:30 H37

Interplay between nanostructure and mechanical properties in natural and artificial polymer fibers — •Periklis Papadopoulos, Roxana Ene, and Friedrich Kremer — Universität Leipzig, Institut für Experimentelle Physik I

The comparison of mechanical with infrared spectroscopy can be used to explore the multi-level nanostructure of semi-crystalline polymers. In this study we attempt to determine the interconnection of the nanocrystal and amorphous phases in two states of spider dragline silk, native and supercontracted with water, and compare it with artificial systems, such as polyamide 6. Crystal stress can be measured with a high time resolution through the analysis of frequency shifts of absorption bands, while varying mechanical fields are applied. The results show that in both states of silk a serial arrangement between the crystalline and amorphous phase dominates the nanostructure. Polyamide 6 films and electrospun fibers have a similar morphology. In silk, however, water can break the hydrogen bonds of the amorphous chains, and, in combination with hydrophobic effects, it induces the formation of a physical network in the amorphous phase. This network increases in stiffness, until a stress limit is reached. At higher stress, the nanostructure of supercontracted silk is irreversibly transformed to one similar to native silk. This enables one to make a complete description of the mechanical properties of silk in both states, by taking into account the energy required to break these bonds in the previous structural model that assumed a pre-strain distribution of worm-like amorphous chains.

CPP 22.3 Wed 14:45 H37

Interplay between morphology and mechanical properties of silk investigated by X-ray microdiffraction on single fibers combined with *in situ* tensile tests — Florian Kunze[1], Igor Krasnov[1], •Christina Krywka[1], Martin Müller[2], Malte Ogurreck[2], Manfred Burghammer[3], and Christian Riekel[3] — [1]IEAP der CAU, Kiel, Germany — [2]GKSS Forschungszentrum, Geesthacht, Germany — [3]ESRF, Grenoble, France

Silk is a natural composite material known to have special mechanical properties. Produced by the silkworm (*Bombyx mori*) it provides high tensile strength and elasticity combined with low weight. It is extremely stretchable with a high degree of toughness and great elongation before breaking. It would be highly desirable to produce artificial fibers with such mechanical properties. Silk fibers have a semicrystalline morphology, which means they are composed of a crystalline and a disordered phase. To determine the characteristics of the mechanical properties and the composition of the silk fibers we are using a combination of *in situ* tensile tests and X-ray microdiffraction. Utilizing the Microfocus Beamline ID13 at the European Synchrotron Radiation Facility (ESRF) it was possible to execute first Wide Angle X-Ray Scattering (WAXS) measurements combined with *in situ* stretching experiments on single silk fibers. The detected effects are similar to those of measurements on small bundles of silk fibers. Overall we have observed a strong interplay between the morphology of silk and the fibers‘ mechanical properties.

CPP 22.4 Wed 15:00 H37

SANS on Silkworm Silk under Tensile Stress — •Malte Blankenburg, Martin Müller, and Melissa Sharp — GKSS Research Centre Geesthacht, Germany

Natural silks exhibit extraordinary mechanical properties, combining high tensile strength with a high elongation at failure. Due to their remarkable mechanical properties and potential medical applications the ability to synthesize silk is still a matter of debate. Silkworm silk fibroin is a semicrystalline nanocomposite, with ordered regions (β-sheet protein nanocrystals) embedded in a softer, amorphous matrix of disordered material [1]. Therefore the contrast between matrix and crystallites could be improved for neutron experiments by deuterating the silk. SANS experiments performed *in situ* during tensile stretching experiments at the SANS-2 instrument at the GKSS showed a peak in the meridional direction of the scattering pattern of deuterated silkworm silk. Since this peak moves to lower q-values by stretching the fibres, an enlargement of the scattering structure could be observed. It was shown before in X-ray experiments [2], that the crystals in the matrix are stretched proportionally to the applied external tensile stress but by a factor of 4 to 18 less than the macroscopic strain. As the percentage elongation is nearly the same for fibre and scattering structure, the scattering objects are not the crystals but rather the ensemble of crystals and disordered material in a periodic arrangement, reflecting the mean distance between crystals in fibre direction.

[1] Y. Shen *et al.*; Macromolecules **31** (1998), 8857
[2] I. Krasnov *et al.*; Phys. Rev. Lett. **100** (2008), 048104

CPP 22.5 Wed 15:15 H37

Rheological properties of wheat dough and corresponding model systems — •Birgitta Schiedt and Thomas Vilgis — Max-Planck Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz,

Wheat dough is a complex material exhibiting non-linear rheological properties, whose underlying molecular origin is still not fully understood. To dumb it down, the macropolymer gluten (protein) present in wheat flour, forms upon hydration and energy input (kneading) an elastic network, into which starch granules are embedded as filler particles. In order to gain more information about the dough formation process as well as the influence of network (protein) - filler (starch) interactions on the overall behaviour of the dough, rheological measurements and microscopy studies are conducted.

The systems investigated include natural wheat dough made from flour and water at different water contents as well as artificial model dough. The latter consists of gluten and various amounts of starch or other filler particles such as glass beads or silica with different chemical surface modifications. The resulting different types of interactions between the starch and filler particles provide deeper insight about the physics of the temporary network.

15 min. break

CPP 22.6 Wed 15:45 H37

Influence of humidity on casein films - an in situ investigation with a combination of μGISAXS and imaging ellipsometry — •Volker Körstgens[1], Robert Meier[1], Johannes Wiedersich[1], Jan Perlich[2], Stephan Volkher Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München Physikdepartment LS E13, James-Franck-Str. 1, D-85747 Garching — [2]HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg

Glues based on casein are known since ancient Egypt. Nowadays casein-based adhesives are being used in versatile labeling applications. Already pure casein shows adhesive properties depending on humidity as shown with tack experiments in this work. The structural changes of thin casein films are investigated in situ with a combination of μGISAXS (grazing incidence small angle x-ray scattering with a μm-sized beam) and imaging ellipsometry. With this new instrument [1] built up at HASYLAB, DESY, Hamburg, 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. Swelling and drying cycles with casein thin films are performed in situ and the relation between structure and adhesive properties is discussed.

[1] V. Körstgens et al., Anal. Bioanal. Chem., DOI 10.1007/s00216-009-3008-1

This project is financially supported by BMBF grant 05KS7WO1.

CPP 22.7 Wed 16:00 H37

Biofunctionalization of Diamond Microelectrodes — •Andreas Adam Reitinger[1], Naima Aurelia Hutter[2], Simon Quartus Lud[1], Gerhard Richter[2], Rainer Jordan[2], Martin Stutzmann[1], and Jose Antonio Garrido[1] — [1]Walter Schottky Institut, TU München, Germany — [2]WACKER-Chair of Macromolecular Chemistry, TU München, Germany

In this work we present two main routes for the biofunctionalization of nanocrystalline diamond films, aiming at the application of diamond microelectrodes as amperometric biosensors. We report on direct covalent grafting of biomolecules on nanocrystalline diamond films via diazonium monophenyls and biphenlys as well as other linker molecules, forming self-assembled monolayers on the diamond surface. Monolayers with different functional head groups have been characterized. Patterning of the available functional groups using electron beam-induced chemical lithography allows the selective preparation of well-localized docking sites for the immobilization of biomolecules. Furthermore, polymer brushes are expected to enable novel paths for designing more advanced biosensing schemes, incorporating multifunctional groups and a higher loading capacity for biomolecules. Here, we will focus on the preparation of polymer grafts by self-initiated photografting and photopolymerization. Further chemical modification of the grafted polymer brushes results in the introduction of additional functional molecules, paving the way for the incorporation of more complex molecular structures such as proteins. In a comparative study we investigate the advantages and disadvantages of both approaches.

CPP 22.8 Wed 16:15 H37

Real-time in-situ study of oligo(ethylene glycol) reordering dynamics and immersion effects using PMIRRAS — •Stefan Zorn, Alexander Gerlach, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Germany

Owing to their high importance in biological and medical applications, e.g. as tethering group for specific binding or, importantly, for passivation of surfaces against unspecific protein absorption, oligo(ethylene glycols) have been the subject of extensive studies. SFG and IR studies revealed strong interactions of water and SAM and strong conformational changes [1]. However, the exact mechanism of protein repulsion is still not fully understood. Here we present a real-time in-situ study of the reordering of the SAM structure during its growth in solution. Using a home build liquid cell with a very thin solution layer (ca. 1 um) we were able to monitor changes in conformation in real time in aqueous environment. With increasing surface coverage there is a change from an amorphous structure with mixed all-trans und helical conformation to a high ordered structure with predominantly helical conformation. A comparison with spectra measured in air shows differences in conformation due to the interaction with water which are more pronounced for lower surface coverage. We also monitored the stability of the SAM over long periods of time and the change in conformation with increasing temperature in solution. Our results shed new light onto the role of water on the structure and protein resistance of OEG SAMs and help to explain the conflicting results in various recent studies.

[1] M.W.A. Skoda et al., Langmuir 23 (2007) 970.

CPP 22.9 Wed 16:30 H37

Protein-resistant polymer coatings based on surface-adsorbed poly(aminoethyl methacrylate)/poly(ethylene glycol) copolymers — •Leonid Ionov[1], Alla Synytska[1], Elisabeth Kaul[1], Stefan Diez[2], and Manfred Stamm[1] — [1]Leibniz-Institut fuer Polymerforschung Dresden e.V., Dresden, Germany — [2]Max-Planck-Institute of Molecular Cell Biology and Genetics, Dresden, Germany

We report on the protein-resistant properties of glass substrates coated with novel copolymers of 2-aminoethyl methacrylate hydrochloride and poly(ethylene glycol) methyl ether methacrylate (AEM-PEG). In comparison to currently available protein-blocking polymer systems, such as poly-L-lysine - poly(ethylene glycol), silane-based poly(ethylene glycol) and poly(ethylene glycol) brushes prepared by surface-initiated polymerization, the proposed AEM-PEG offers the combined advantages of low cost, simplicity of use and applicability in aqueous solutions. We demonstrate the capability of AEM-PEG to block the surface binding of globular proteins (tubulin), their assemblies (microtubules) and functional motor proteins (kinesin-1). Moreover, we demonstrate the applicability of AEM-PEG for surface patterning of proteins in microfluidic devices.

CPP 22.10 Wed 16:45 H37

Protein folding monitored at six different magnetic field strengths — •Michael Kovermann and Jochen Balbach — Institut für Physik/Fachgruppe Biopyhsik, Martin-Luther-Universität Halle-Wittenberg, Betty-Heimann-Straße 7, D-06120 Halle/Saale, Germany

The folding mechanism of an elongated polypeptide chain into its native three dimensional structure is still of high common interest. Using NMR spectroscopy we are able to follow the permanently occuring folding and unfolding of the cold shock protein B from Bacillus subtilis, *Bs*CspB, in equilibrium and kinetically on a ms timescale.

So-called NMR relaxation dispersion experiments are able to monitor these dynamic events on a ms - to - μs timescale at atomic resolution. We performed these kind of experiments at six different magnetic field strengths to get reliable results. As the folding (and the unfolding) rate of a protein should be independent of the external magnetic field strength we fitted this kinetic parameter in a global procedure to the NMR relaxation data. In addition to these folding rates we get out structural and thermodynamic information by these dynamic NMR experiments.

Topical Talk CPP 22.11 Wed 17:00 H37

Recognition dynamics and kinetics for ubiquitin — •Christian Griesinger — MPI for Biophysical Chemistry, Goettingen, Germany

We measured residual dipolar couplings in a large number of alignment media for ubiquitin and derived an ensemble with the EROS method that reflects motion up to the microsecond time scale. The ensemble fits very well the NMR parameters used for the refinement and cross validates other unused NMR parameters such as J-couplings and other dipolar couplings. The ensemble has an rmsd of approximately 1Åand shows large fluctuations in loops as well as in secondary structure elements. The ensemble reflects mainly motion on the previously inaccessible time scale between ns and microseconds. Its implications for molecular recognition will be discussed. We have further measured the time scale of the recognition dynamics and find a previously unobservable sub-β-peak in dielectric relaxation spectroscopy in solution that can be explained by a modulation of the ion conductance by the conformational ensemble. From the temperature dependence of this effect, on can expect to slow down the dynamics in supercooled solution to approximately 50 μs. Indeed, relaxation dispersion measurements in supercooled solution reveal that the time scale of major conformational interconversions is 50 to 100 μs and that the above mentioned ensembles predict correctly the relaxation dispersion data. Furthermore, correlated motion in the ensemble has been quantified experimentally with cross correlated relaxation. We find that the above mentioned rdc derived ensembles agree much better with the cross correlated relaxation data than ensembles that reflect only individual motion.

CPP 23: Polymer Dynamics

Time: Wednesday 9:30–12:45 Location: H48

Invited Talk CPP 23.1 Wed 9:30 H48

On the dynamics of polymers in nanocomposites and under confinement — •Dieter Richter — Jülich Centre for Neutron Science and Institute for Solid State Research, Research Center Jülich, D-52425 Jülich, Germany

Confinement effects in polymer melts may lead to unusual properties. This concerns both, the chain conformation as well as chain dynamics that may be altered due to the surface interactions and changes of topology. In my presentation I will display neutron scattering data, addressing length and time scales from the single monomer to the entanglement network and beyond. These experiments reveal the basic relaxation rates related to monomeric friction, the intermediate scale Rouse dynamics as well as the entanglement controlled dynamics. Polymer nanocomposites have been investigated at various compositions using filler particles smaller and larger than the polymer size. I will discuss the effects of the filler size and concentration on the polymer conformation as well as on the dynamics on the various important length scales. The effect of confinement was also studied on well defined porous alumina samples which were filled with polyethylene oxide (PEO). Thereby the chain dimensions were much larger or smaller than the lateral pore size D. While for the long chains an expanded entanglement network is observed, the confinement seems to have a weaker effect on the short chains. In particular we do not observe any corset effect as proposed by NMR relaxometry.

Topical Talk CPP 23.2 Wed 10:00 H48

From simple liquids to polymers: Dynamics revealed by field cycling ^{1}H NMR — Axel Herrmann, Azza Abou Elfadl, Roman Meier, Danuta Kruk, Vladimir N. Novikov, and •Ernst A. Rössler — Experimentalphysik II, Universität Bayreuth, 95440 Bayreuth, Germany

We apply field cycling NMR to study the crossover from glassy through Rouse to reptation dynamics in series of different linear polymers (PB, PDMS, PPO, PI) with molecular weight M ranging from the low-M limit (simple liquid) to the high-M limit. Dispersion data of the spin-lattice relaxation time $T_1\,(\omega)$ are transformed to the susceptibility representation $\chi''\,(\omega\tau_s) = \omega/T_1$, and using frequency-temperature superposition master curves $\chi''\,(\omega\tau_s)$ (τ_s:= segmental correlation time) are constructed which reflect spectral contributions from glassy as well as polymer specific dynamics. We are able to cover six decades at $\omega\tau_s < 1$ allowing to monitor in detail the emergence of polymer specific relaxation contributions. Transforming the master curves into the time domain yields the segmental reorientational correlation function which we follow over six decades in amplitude. From this the order parameter as well as bond-vector correlation function are derived. Comparison with theoretical predictions by the tube-reptation model as well as renormalized Rouse theory reveals significant discrepancies whereas good agreement is found with Monte Carlo simulations. We conclude that the crossover to entanglement dynamics appears to be highly protracted. This is confirmed by accompanying measurements of dielectric normal mode spectra.

CPP 23.3 Wed 10:30 H48

Bond-correlation functions determined in MD simulations of entangled polymer melts — •Hendrik Meyer — Institut Charles Sadron, CNRS UPR22, 67034 Strasbourg, France

The polymer dynamics of entangled bead-spring chains is analysed based on large scale molecular dynamics simulations. As found in previous studies, the predicted power law regimes of mean-square displacements attributed to Rouse-motion in the tube (cross-over from $t^{0.5}$ to $t^{0.25}$) are only well developed beyond $Z \geq 10$ entanglements per chain. Similar power law regimes are present for bond time-autocorrelation functions ($P_1 \propto t^{-0.5}$ and $t^{-0.25}$). NMR experiments measure a correlation function proportional to the second Legendre polynomial P_2 of the bond correlations, which is found to be proportional to the square of P_1 only for flexible chains, whereas a slower time decrease is found for chains with a small angular potential. Clear evidence is found that the terminal relaxation time increases stronger than predicted by reptation theory for $Z > 5$. We critically compare this finding with theories of contour length fluctuations, often invoked as the main explanation of this slowing down.

15 min. break

CPP 23.4 Wed 11:00 H48

The role of the intermolecular magnetic dipole-dipole interaction in low frequency proton NMR in polymer melts. — •Nail Fatkullin[1], Anvar Gubaidullin[1], Siegfried Stapf[2], and Rainer Kimmich[3] — [1]Kazan State University, Kazan 420008, Tatarstan, Russia — [2]Technische Universität Ilmenau, Dept. Technical Physics II, 98684 Ilmenau, Germany — [3]University of Ulm, Sektion Kernresonanzspektroskopie, 89069 Ulm, Germany

The different contributions to the dynamic magnetic dipole-dipole correlation function, which is responsible for proton NMR phenomena like the spin-lattice relaxation, the free induction decay, the solid echo, etc.„ are analyzed. For the anisotropic tube-reptation model the relative weight of the intra-molecular contribution in the time dependent magnetic dipole-dipole correlation function should progressively increase with time, corresponding to lower resonance frequency, compared to the intermolecular contribution. For the isotropic n-Renormalized Rouse model the situation is opposite: with increasing of time/decreasing frequency the relative weight of the intermolecular contribution progressively increases and may eventually dominate. Theoretical estimations and analyses of published experimental results, connected with proton NMR spin-lattice relaxations in polymer melts, directly show that at times longer than and at frequencies below the regime, neglecting the intermolecular contributions to proton NMR phenomena in polymer melts, as had been done in the majority of scientific papers, is incorrect.

CPP 23.5 Wed 11:15 H48

Multiple quantum NMR observation of reptation and constraint release in polymer melts — •Fabian Vaca Chavez and Kay Saalwaechter — Institute of Physics, Martin-Luther-University Halle-Wittenberg, Halle (Saale), Germany

In his seminal paper, de Gennes [1] propose a qualitative explanation of the polymer melts dynamics, far above the entanglement molecular weight Me, in terms of a reptative, snake-like motion of the chain through a mesh of fixed topological constraints (entanglements) set by the other chains. Here we show results from 1H multiple quantum (MQ) NMR on a benchtop spectrometer [2], probing the validity of the tube model of polymer dynamics, which combines the reptation concept with the Rouse theory for unentangled chains. This fixed-tube model is insuficient for the quantitative description of actual mechanical data, and ongoing discussions focus on including dynamics of the tube itself, caused by contour-length fluctuations (CLF), arising from chain-end motions of the test chain, or constraint release (CR), arising from matrix chain motions. We also observe characteristic deviations from the tube model predictions up to high molecular weights, and show that CR processes are responsible for modified chain modes faster than actual reptation. Our results extend previous observations by neutron spin-echo spectroscopy (NSE), whose limited dynamic range poses limitations to the study of well-entangled systems.

[1] P. G. de Gennes, J. Chem. Phys., 55, 572 (1971). [2] K. Saalwaechter, Progr. NMR Spectrosc., 51, 1 (2007).

CPP 23.6 Wed 11:30 H48

Atomistic molecular dynamics simulations of polybutadiene at graphite: slowing down of orientation relaxations in confinement vs. bulk system — •Leonid Yelash[1], Peter Virnau[1], Wolfgang Paul[2], and Kurt Binder[1] — [1]Institut für Physik, Johannes-Gutenberg Universität Mainz — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg

A nanoscopic thin polybutadiene film confined between two graphite surfaces is studied using molecular dynamics simulations. Polymer is described with an united atom model incl. Lennard-Jones, bending and torsion interactions[1]. The crystalline surface is modeled by several layers of graphite atoms placed at their crystallographic positions[2]. Our previous study has shown that the confinement affects the statics as well as the dynamics. E.g., gyration radius calculated perpendicular to the surface decreases strongly near the surface showing that the whole molecules prefer to orient parallel to the surface. The mean square displacement shows a preferred lateral diffusion of polymer; the diffusion perpendicular to the surface is significantly slowed down.

Here we report results of our recent analysis of the MD data for the orientation relaxations of specific chemical bonds (α-, β-, and double-bonds) present in polybutadiene as well as dielectric relaxation in bulk and confined systems. Such relaxation functions can be obtained experimentally, e.g., from NMR measurements[3].

[1] Smith, G.D., and Paul, W., *J. Phys. Chem. A*, *102*, 1200 (1998); Krushev, S., *Diss.* Mainz 2002. [2] Steele, W.A., *Surf. Sci.*, *36*, 317 (1973). [3] Saalwächter, K., *Prog. NMR Spec.*, *51*, 1 (2007)

CPP 23.7 Wed 11:45 H48

Understanding the Origin of Dynamical Heterogeneities in Polymer Blends — •Diddo Diddens[1,2], Andreas Heuer[1,2], and Martin Brodeck[3] — [1]Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 30, 48149 Münster, Germany — [2]NRW Graduate School of Chemistry, Corrensstraße 36, 48149 Münster, Germany — [3]Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Polymer blends composed of poly(ethylene oxide) (PEO) and poly(methyl methacrylate) (PMMA) have been the focus of many investigations such as neutron scattering or NMR experiments. Within this polymer blend both components have greatly different glass transition temperatures, so that the low-T_g compound (PEO) moves in a random, nearly frozen environment imposed by the high-T_g compound (PMMA), leading to strong dynamical heterogeneities within the PEO dynamics. One common approach to model the dynamics of the PEO chains is the phenomenological Random-Rouse Model, in which the random environment imposed by the slow PMMA component is modelled by a Rouse chain with different friction coefficients on each bead.

Here we discuss the merits and limitations of the Random-Rouse Model for a simulated PEO/PMMA blend. By using a recently developed method to determine local mobilities in polymeric systems, we can check the different assumptions of this model. Moreover, the length-scale dependence of the retardation of the PEO dynamics in the blend compared to the homopolymer was studied.

CPP 23.8 Wed 12:00 H48

Investigation of structural heterogeneities of porous diblock copolymer membranes by single particle tracking — •Chandrashekara R. Haramagatti[1], Dominique Ernst[1], Felix Schacher[2], Mathias Ulbricht[3], Axel H. E. Müller[2], and Jürgen Köhler[1] — [1]Experimental Physics IV, University of Bayreuth, 95440, Bayreuth, Germany — [2]Macromolecular Chemistry II, University of Bayreuth, 95440, Bayreuth, Germany — [3]Technical Chemistry II, University of Duisburg-Essen, 45117, Essen, Germany

We study the structural heterogeneity of porous diblock copolymer membranes employing single particle tracking. The membranes were prepared by non solvent induced phase separation (NIPS) methods. Information on the thickness and pore sizes of the membranes is known from scanning electron microscopy. Fluorescent polystyrene beads were used as fluorescent particles and the spatial position of which was monitored with sub-diffraction limited accuracy. The diffusion behavior of these particles provides information of the structural properties of the membranes.

CPP 23.9 Wed 12:15 H48

Dynamics in thin polymer films probed by single molecule fluorescence microscopy at high temperatures — •Bente Flier, Moritz Baier, Johannes Huber, Dominik Wöll, Stefan Mecking, and Andreas Zumbusch — Fachbereich Chemie, Universität Konstanz, Universitätsstraße 10, 78457 Konstanz, Germany

Wide-field fluorescence microscopy is a versatile technique for the investigation of single molecule dynamics. We use this technique for the analysis of dynamical properties of thin polymer films in the vicinity of the glass transition temperature. In this contribution we present first results of high temperature single molecule studies above 400 K of polystyrene and poly butyl methacrylate films with thicknesses between 10 nm and 100 nm. For single molecule measurements fluorescent dyes are either covalently bound to the polymer chains or used as probes of free volume. The measurements yield the temperature dependence of the diffusion coefficients which can be explained by free-volume theory. Compared to bulk techniques, however, the single molecule approach allows for an investigation of diffusional heterogeneities.

CPP 23.10 Wed 12:30 H48

Dynamics of semiflexible treelike polymeric networks — •Maxim Dolgushev and Alexander Blumen — Theoretische Polymerphysik, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Deutschland

Extending the generalized Gaussian structure model[1] we study the dynamics of treelike networks, in which we include stiffness using mean-field restrictions on the bonds' orientations. We proceed by using the Bixon-Zwanzig-model[2] and also the maximum entropy principle[3]. For semiflexible treelike networks both approaches turn out to be equivalent[4]. The dynamics of semiflexible treelike polymers obeys Langevin equations, which we succeeded in deriving analytically[4]. This allows us to determine straightforwardly the dynamical characteristics relevant to mechanical and dielectric relaxation[4,5].

[1] A. A. Gurtovenko and A. Blumen, Adv. Polym. Sci., 182, 171 (2005).

[2] M. Bixon and R. Zwanzig, J. Chem. Phys., 68, 1896 (1978).

[3] R. G. Winkler, L. Harnau, P. Reineker, J. Chem. Phys., 101, 8119 (1994).

[4] M. Dolgushev and A. Blumen, J. Chem. Phys., 131, 044905 (2009).

[5] M. Dolgushev and A. Blumen, Macromolecules, 42, 5378 (2009).

CPP 24: Glasses and Glass Transition I (jointly with DY and DF)

Time: Wednesday 14:00–17:30 Location: H48

Invited Talk CPP 24.1 Wed 14:00 H48

New Approach to the Old Problem: Cooperativity in Dynamics of Glass Forming Systems — •Alexei Sokolov — Oak Ridge National Lab and UT Knoxville, USA

The mechanism behind the steep slowing down of molecular motions upon approaching the glass transition remains a great puzzle. Most of the theories relate this mechanism to the cooperativity in molecular motion. In this talk we present estimates and analysis of the molecular cooperativity in many glass-forming systems. We demonstrate that the cooperativity length scale directly correlates to the dependence of the structural relaxation on volume. This dependence presents only one part of the mechanism of slowing down the structural relaxation. Our analysis reveals that another part, the purely thermal variation of the structural relaxation, does not have a direct correlation with molecular cooperativity. These results call for a conceptually new approach to the analysis of the mechanism of the glass transition and to the role of molecular coopertaivity in slowing down of structural relaxation.

CPP 24.2 Wed 14:30 H48

THz Signatures of the Glass Transitions in Polymers — •Marco Reuter[1], Steffen Wietzke[2,3], Christian Jansen[2,3], Tilmann Jung[1], Sangam Chatterjee[1], Wiebke Dempwolf[4], Henning Menzel[4], and Koch Martin[1,3] — [1]Fachbereich Physik, Philipps-Universität Marburg, Renthof 5, 35032 Marburg, Germany — [2]Institut für Hochfrequenztechnik, TU Braunschweig, Schleinitzstr. 22, 38106 Braunschweig, Germany — [3]Joint Optical Metrology Center, c/o TU Braunschweig, Fakultät für Elektrotechnik und Informationstechnik, Hans-Sommer-Str. 66, 38106 Braunschweig, Germany — [4]Institut für Technische Chemie, TU Braunschweig, Hans-Sommer-Str. 10, 38106 Braunschweig, Germany

The glass transition temperature of polymers is found with terahertz time-domain spectroscopy. In the region of the glass transition the thermo-quasi-optic coefficient changes noticeably. THz time-domain spectroscopy is a non-destructive and non-contact technique to analyse polymers.

CPP 24.3 Wed 14:45 H48

The elusive nature of the Debye process in monohydroxy alcohols: A new approach with ^{2}H-NMR techniques — •Sebastian Schildmann, Catalin Gainaru, and Roland Böhmer — Experimentelle Physik III, Fakultät für Physik, Technische Universität Dortmund

Viscous monohydroxy alcohols, also water, exhibit a so called Debye process in their dielectric spectra. This relaxational feature corresponds to degrees of freedom which are about 100 times slower than those giving rise to the structural rearrangements (α-process). In spite of numerous experimental investigations [1], the nature of these slow "superstructure" relaxation modes is not agreed upon, although it is clear that they are to be related with the presence of hydrogen bonds. The Debye process separates from the structural process if the network is interrupted chemically by diluting or topologically by confining the system in pores. Here butanol diluted with bromobutane was studied with several ^{2}H-NMR techniques. Correlation times measured with stimulated-echo experiments are compared with data obtained from dielectric spectroscopy [2]. Spin-lattice relaxation times were measured for O-D deuterated samples to check how the hydrogen bonds affect the dynamics.

[1] M. Poeschl & H.G. Hertz, J. Phys. Chem. 98, 8195 (1994).

[2] T. El Goresy & R. Böhmer, J. Chem. Phys. 128, 154520 (2008).

CPP 24.4 Wed 15:00 H48

Relaxation Kinetics of Nanoscale Indents in a Polymer Glass — •Armin Knoll, Dorothea Wiesmann, Bernd Gotsmann, and Urs Duerig — IBM Research - Zurich, 8803 Rueschlikon, Switzerland

Nanometer scale indents have been written in a cross-linked polystyrene sample, and their relaxation has been studied at annealing temperatures well below the glass transition of the polymer. The indents represent a highly nonequilibrium state of the polymer which is subjected to mechanical stress of up to 0.4 GPa and thermal quench rates on the order of 10^8 K/s during writing. It is shown that the relaxation towards equilibrium evolves logarithmically over more than 10 orders of magnitude in time. The relaxation kinetics are accurately described in terms of a thermally activated process with an energy barrier whose magnitude decreases linearly with the distance from equilibrium [1].

[1] A. Knoll, D. Wiesmann, B. Gotsmann, and U. Duerig, *Phys. Rev. Lett.*, **102**, 117801 (2009)

CPP 24.5 Wed 15:15 H48

Studying the dynamics of water molecules on a complex lattice: KOH doped tetrahydrofuran clathrate hydrate — •Helge Nelson[1], Catalin Gainaru[1], Andre Nowaczyk[1], Sebastian Schildmann[1], Burkhard Geil[2], and Roland Böhmer[1] — [1]Experimentelle Physik III, Fakultät für Physik, TU Dortmund — [2]Institut für Physikalische Chemie, Universität Göttingen

Because of kinetic hindrance during the freeze-out of the protons in clathrate hydrates an orientational glass transition is observed. By adding minute amounts of ionic dopants, e.g., KOH, the timescale of ordering can be accelerated significantly and an ordered phase is reached [1]. We applied a combination of dielectric and ^{2}H-NMR techniques to study the lattice dynamics of the water molecules in a temperature range from 30 K to 260 K. The ^{2}H-NMR techniques include temperature dependent lineshape analysis, measurement of relaxation times, and the stimulated-echo technique. This combination allows the observation of dynamics in a broad frequency and temperature window. We found several reorientational processes on the lattice, which are absent in the undoped sample. In addition we were able to detect the phase transition into the proton ordered phase with both dielectric and NMR measurements close to 62 K.

[1] see O. Yamamuro, et al., Physica B 213, 405 (1995) and references cited therein.

15 min. break

Invited Talk CPP 24.6 Wed 15:45 H48

Slow domains percolation in polymer melts and blends close to the glass transition: a unifying concept regarding bulk dynamics, dynamics in the vicinity of interfaces, and the physical properties of nanocomposites — •Didier R. Long — Laboratoire Polymères et Matériaux Avancés; CNRS/Rhodia; F-69192 Saint Fons, France.

Experiments have demonstrated over past 15 years that the dynamics in liquids close to and below the glass transition temperature is strongly heterogeneous, on the scale of a few nanometers and, independantly, that the glass transition temperature in the vicinity of interfaces can be very different from that in the bulk, with shifts either positive or negative depending on the interaction between the polymer and the interface. By considering thermally induced density fluctuations in the bulk, we proposed that the 3-D glass transition is controlled by the percolation of small domains of slow dynamics, which allows to explain the heterogeneous dynamics close to Tg. This model allowed then for interpreting a priori unrelated features of polymer dynamics: 1) the main feature of confinement effects on the dynamics; 2) Unique reinforcement, plastic and recovery behaviour of nano-filled elastomers; 3) ageing and rejuvenating dynamics polymeric liquids; 4)case II diffusion, which is how a solvent penetrates and finally melts a glassy polymer matrix.

Regarding these various issues, I will put the emphasis on how percolation of slow domains is key for explaining their main features.

CPP 24.7 Wed 16:15 H48

Glass Transition of Molecules Sorbed in Zeolites — Özlen F. Erdem[1], •Dieter Michel[2], Pavel Sedykh[2], and Jürgen Haase[2] — [1]Max-Planck-Institute of Bioinorganic Chemistry, Stiftstraße 34-36, 45470 Mülheim an der Ruhr, Germany — [2]University of Leipzig, Faculty of Physics and Earth Sciences, Linnéstraße 5, 04103 Leipzig, Germany

Proton MAS NMR, nuclear spin relaxation, and deuteron NMR spectroscopy are combined to study the mobility of ethylene glycol molecules sorbed in various zeolites over a wide temperature range. The results obtained will be also compared with broad-band dielectric measurements and with previous extensive dielectric studies by Kremer *et al.* [1]. The main question is whether the adsorbed species show a so called single-molecule behavior characterized by an Arrhenius type temperature dependence of the correlation times or the respective dielectric relaxation times. In contrast, a Vogel-Fulcher-Tammann (VFT) type temperature dependence of the dielectric relaxation rate would point out collective motions and is typical for the appearance of a glass-transition. An important question is the competition between molecule-to-molecule and molecule-to-surface interactions.

[1] F. Kremer, A. Huwe, M. Arndt, P. Behrens, W. Schwieger, J. Phys. Cond. Mat. **11**, A175-A188 (1999); A. Huwe, F. Kremer, J. Kärger, P. Behrens, W. Schwieger, G. Ihlein, O. Weiss, F. Schuth, J. Mol. Liquids **86**, 173-182 (2000).

CPP 24.8 Wed 16:30 H48

Molecular glass formers in hard and soft confinement probed by ^{31}P and ^{2}H NMR — •Daniel Bock, Sabine Gradmann, and Ernst Rössler — Experimentalphysik II, Universität Bayreuth

Low molecular glass formers confined in nanoporous silica matrices (hard confinement) are investigated by different ^{31}P and ^{2}H NMR methods such as spin-lattice-, spin-spin relaxation, line-shape and stimulated echo decay.

Decreasing the radius of the pores pronounced dynamic heterogeneities are observed. For example, the correlation function revealed by the stimulated echo exhibits a quasi-logarithmic decay in contrast to Kohlrausch decay in the bulk. As shown by 2D spectra the dynamic heterogeneities are transient in time, i.e., we observe exchange between slow and fast molecules. The effects are explained by assuming dynamics being inhomogeneous in space; that is the dynamics given by a correlation time $\tau(r)$ depend on the distance r from the confining wall.

Similar NMR features are found for low molecular additives dissolved in polymer matrices (soft confinement). The additive dynamics are decoupled from those of the polymer, and liquid-like additive dynamics are revealed below T$_g$, i.e., in a solid polymer matrix. Again, strongly stretched correlation functions are observed.

CPP 24.9 Wed 16:45 H48

Quantitative Lineshape Analysis for 1D- and 2D-Spectra of Amorphous Materials — •Jörn Schmedt auf der Günne, Sabarinathan Venkatachalam, Johannes Weber, and Yamini Avadhut — Department of Chemistry, Munich University (LMU), Germany

NMR is quantitative, is an often stated feature in magnetic resonance. In ^{1}H solid-state NMR the results from simple MAS experiments can be disappointing though. We present a model study [1] which identifies and quantifies different sources of errors and a new strategy which gives reliable results even under low resolution conditions.

A second aspect will be 2D deconvolution of the lineshapes of amorphous/glassy materials. We analyze the unexpected splittings in the 2D lineshape of many typical glasses with a new analytical fitting function. Based on these findings we suggest a structural model based on different subunits, which should also find their imprint in bulk properties.

[1] Y.S.Avadhut, D.Schneider, J.Schmedt auf der Günne, J. Magn. Reson. 201 (2009) 1-6.

CPP 24.10 Wed 17:00 H48

Low-Frequency Excess Contribution in Simple Liquids Revealed by Fast Field Cycling NMR — •Roman Meier, Axel Herrmann, Robert Kahlau, Danuta Kruk, and Ernst Rössler — Experimentalphysik II, Universität Bayreuth, Germany

The main relaxation (α-relaxation) of simple liquids studied by dielectric spectroscopy is well described by a Cole-Davidson (CD) susceptibility. In particular the low-frequency limit follows a Debye behavior $\chi''_{DS} \propto \omega^1$. Applying fast field cycling (FFC) ^{1}H NMR and transforming the spin-lattice dispersion data T_1 into the susceptibility representation $\chi''_{NMR} \propto \nu/T_1$ we have discovered a low-frequency excess contribution for systems like glycerol and its homologues as well as fluoroaniline. The CD function fails to describe the data due to a retarded transition to the limit ω^1, i.e., a "shoulder" is observed on the low frequency side of the a-relaxation peak ($\omega\tau_\alpha < 1$) possibly reflecting a slower relaxation process. Actually only a few liquids like o-terphenyl and tristyrene studied by FFC NMR do not show this phenomenon. Collecting dispersion data over a large temperature range, the relaxation strength of the excess contribution is specified quantitatively. Measurements of dilution series of propylene glycol in deuterated chloroform proved an intermolecular origin of the excess contribution. Dilution experiments of deuterated in protonated glycerol suggest this additional contribution being also fully reflected by sole intramolecular spin-spin vectors. A possible explanation of this effect are transient molecular clusters due to chemical interactions (e.g. H-bonds).

CPP 24.11 Wed 17:15 H48

Glass transition of colloidal particles with long-ranged interactions in two dimensions — •David Hajnal, Martin Oettel, and Rolf Schilling — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany

We study the glass transition behavior of binary mixtures of colloidal particles with long-ranged dipolar interactions in two dimensions in the framework of mode-coupling theory (MCT). We first present a minimal model for the theoretical description of the thermodynamic properties of the experimental system studied by König et al. [1]. By applying MCT to this model, we determine its glass transition diagram, i.e. we calculate the variation of the critical interaction strength upon composition changes. Finally, we compare the mixing effects predicted by MCT for this model to both experiments [1] and MCT results for binary mixtures of hard disks [2].

[1] H. König, R. Hund, K. Zahn, and G. Maret, Eur. Phys. J. E **18**, 287 (2005).

[2] D. Hajnal, J. M. Brader, and R. Schilling, Phys. Rev. E **80**, 021503 (2009).

CPP 25: Focus: Active Fluids

Time: Wednesday 9:30–12:30 Location: H39

Invited Talk CPP 25.1 Wed 9:30 H39

Designing small swimmers — •Ramin Golestanian — Department of Physics and Astronomy, University of Sheffield, Sheffield, UK

The directed propulsion of small scale objects in water is problematic because of the combination of low Reynolds number and strong thermal fluctuations at these length scales. One possibility for designing propulsion is to devise non-reciprocal deformation strategies that are simple enough to be realizable. This opens up the discussion of what is the minimum number of degrees of freedom that we can use in our design strategies for objects that can swim at low Reynolds numbers. We introduce a simple prototype of a model based on a linear assembly of three spheres that are attached by two flexible linkers that can change their lengths. We analyze the motion of this model swimmer both in the deterministic and stochastic regimes. Another strategy to achieve propulsion at low Reynolds numbers could be to take advantage of various phoretic phenomena. We propose a simple model for the reaction-driven propulsion of a small device is proposed as a model for a molecular swimmer in aqueous media. Finally, a number of experimental realizations of such microswimmers are discussed including, in particular, one experiment in Sheffield and another one in Barcelona.

Invited Talk CPP 25.2 Wed 10:00 H39

Magnetic actuation of paramagnetic colloids at interfaces — •Thomas Fischer — University of Bayreuth

Spatio temporal variations of a magnetic field allow the dynamic control of paramagnetic colloids near interfaces. The flux of magnetic energy into the colloidal system renders the colloid into an active fluid. We report on the structure, dynamics, and transport of active two dimensional paramagnetic colloids in magnetic fields that vary on the colloidal scale. Several novel dynamical regimes are observed and reported, from localized trajectories to direct particle transport, depending on the geometry of the underlying magnetic pattern and on the parameters, which control the external driving field, such as frequency, strength and direction.

CPP 25.3 Wed 10:30 H39

Brownian dynamics of a self-propelled particle on a substrate — •Borge ten Hagen[1], Sven van Teeffelen[2], and Hartmut Löwen[1] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Universitätsstr. 1, 40225 Düsseldorf, Germany — [2]Department of Molecular Biology, Princeton University, LTL-343A Washington Road, Princeton, NJ 08544, USA

By solving the Langevin equation analytically, we study the overdamped Brownian motion of a self-propelled particle which is driven by a projected internal force. The "active" particle under study is restricted to move along a linear channel or in a two-dimensional plane. Its orientation, the direction of the internal force, is either freely diffusing on the unit sphere or confined to a plane perpendicular to the substrate. For a subset of the cases considered, the impact of a uniaxial torque and of external potentials is investigated as well. While the basic model applies to spherical particles, a generalized version which holds for ellipsoidal particles is also developed. The model is relevant for active particles like catalytically driven Janus particles and bacteria moving on a substrate. Analytical results for the first four time-dependent displacement moments are presented and analysed for several special situations. A significant dynamical non-Gaussian behaviour at finite times is signalled by a non-vanishing normalized kurtosis.

15 min. break

CPP 25.4 Wed 11:00 H39

Efficiency of phoretic micromotors — •Benedikt Sabass and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart

Small objects, propelled through phoretic surface processes, could be employed for active transport or even as micromotors. A common characteristic of these processes is the generation of a surface flow around the motor by different mechanisms. Here we investigate the thermodynamic properties of phoretic effects. We derive a general expression for the efficiency of motors and show that it is bounded by its hydrodynamic contribution. A general argument is proposed according to which the hydrodynamic efficiency of propulsion mechanisms relying on surface effects scales as L/R where L is the thickness of the interface layer and R is the lengthscale of the object. This finding supports the notion that this class of processes is very often quite inefficient. We also illustrate our findings with concrete examples.

Invited Talk CPP 25.5 Wed 11:15 H39

Active behavior of the cytoskeleton — •Jean-Francois Joanny and Jacques Prost — Institut Curie Centre de Recherche Physico-Chimie Curie 26 rue d'Ulm, 75248 Paris Cedex 05 France

The mechanical properties of cells are dominated by the actin-myosin cytoskeleton. It is a gel-like structure formed by actin filaments which is active and intrinsically out of equilibrium since it contains molecular motors which permanently consume energy in the form of ATP.

We first present a hydrodynamic theory of active polar systems that allows for the description of the mechanical properties of the cytoskeleton. This theory is based on symmetry principles and is thus very similar to the hydrodynamic theories proposed for other active systems at very different length scales (animal behavior, bacterial suspensions...).

We then illustrate this theory by presenting some instablities of cells associated to the cortical actin layer: bleb formation, cell oscillations, contractile ring formation.

Invited Talk CPP 25.6 Wed 11:45 H39

Active cytoskeletal polymer networks: from model systems to cells — •Christoph F. Schmidt — Drittes Physikalisches Institut, Georg-August-Universität Göttingen, Germany

Mechanical processes, such as cell division and growth or cell locomotion, are essential in cell life and are driven and controlled by the cytoskeleton. The polymeric components of the cytoskeleton are semiflexible polymers. Force-generating motor proteins are tightly integrated into these polymer networks which makes the cytoskeleton a prototypical "active gel".

We study mechanical properties and collective dynamics of cells and of in vitro model systems for active cytoskeletal networks with microrheology techniques. We use micron-sized probe particles, embedded in the medium to be studied, and laser optical traps to confine the particles, combined with laser interferometry to detect either their Brownian motion or the particles' response to a driving force with sub-nm accuracy and bandwidths up to 100 kHz. We have applied this technology to non-equilibrium systems and have measured, at the same time, the elastic properties and the fluctuations and forces generated by myosin motor proteins interacting with a cross-linked actin network. We have also applied the same type of approach to several types of cells, and have monitored cellular forces transmitted to externally attached probe particles.

CPP 25.7 Wed 12:15 H39

Active fluids and soft matter in biotechnology and medicine — •Magnus Jaeger — Saarland University, Faculty of Clinical Medicine (2.28), 66421 Homburg / Saar, Germany

Biologically and medically relevant fluids are highly complex. They consist of suspensions containing non-negligible concentrations of deformable particles: cells. The cells have to be (a) identified in mixtures and (b) sorted into individual fractions. Both requirements are fulfilled by different methods commonly employed. However, these methods become inapplicable, if only small sample volumes are available, e. g. a drop of blood. Additional demands comprise disposables, robustness, low costs and quick results in minutes.

We aim at contributing to this crucial topic, based on our expertise in micro- and nanofluidics. We pursue several research approaches: (I) cells can conveniently be identified by their mechanical properties. To this end, we deform them in a harmless electric field. This technique is fast (seconds), simple (integrable into chip systems) and automatable. We clearly distinguished cancer cells from normal cells of the same tissue. (II) Microfluidics depends on the surface properties of materials, e. g. wettability. We investigate effects of coatings with switchable polymers that change their conformation in a sharp, reversible phase transition between a hydrated, elongated state and a dehydrated, collapsed state. The transition can arbitrarily be controlled externally through the temperature. (III) Further issues concern controllably releasing substances from the cells (RNA) and the separation of the macromolecule solutions.

CPP 26: Micro and Nanofluidics I

Time: Wednesday 14:00–17:30 Location: H39

CPP 26.1 Wed 14:00 H39

Sorption in elastically coupled microporous media: Equilibrium and dynamics — •Kristian Müller-Nedebock — Stellenbosch University, Stellenbosch, Südafrika

Microporous materials in which small guest molecules can be sorbed and where pores are coupled elastically are studied. We show how multiple state models with elastic interactions can account for experimentally determined adsorption isotherms. We also present a simple theoretical model for an auxetic medium, consisting of counter-rotating hinged elements, that permits selective sorption of molecules in dependence of shape and size. This tuning can be achieved through the application of external hydrostatic pressure on the host. A mean-field treatment of the model indicates both continuous and first-order phase transitions. Finally, we study simple dynamics of filling of medium of one-dimensional, yet elastically coupled pores, which pose extremely interesting and mathematically challenging problems beyond that of slow single-file diffusion. Here we develop a Langevin equation approach in order to understand better the subdiffusive regime.

CPP 26.2 Wed 14:15 H39

Pore-scale investigations of multiphase fluid systems subject to freeze-thaw — •Kamaljit Singh[1,2,3], Robert K. Niven[1], Timothy J. Senden[4], Michael L. Turner[4], Adrian P. Sheppard[4], Jill P. Middleton[4], and Mark A. Knackstedt[4] — [1]School of Aerospace, Civil and Mechanical Engineering, The University of New South Wales at ADFA, Northcott Drive, Canberra, ACT, 2600, Australia — [2]Max Planck Institute for Dynamics and Self-Organization, D-37018 Göttingen, Germany — [3]Experimental Physics, Saarland University, 66123 Saarbrücken, Germany — [4]Department of Applied Mathematics, Research School of Physics and Engineering, Australian National University, ACT, 0200, Australia

The pore scale behavior of non-aqueous phase liquid (NAPL) contaminants in porous media undergoing freeze-thaw cycles is studied by conducting various experiments, including two-dimensional micromodels, containing residual NAPL in a monolayer of glass beads; and three-dimensional glass-bead cell using X-ray micro-computed tomography. It is shown that freeze-thaw cycles have a substantial impact on the distribution of residual NAPL (in initially water saturated porous media), including the rupture and remobilization of trapped NAPL due to freezing-induced pressure forces, and ganglion fragmentation into singlet ganglia. The results of these experiments are interpreted by developing pore-scale models. The findings have important implications for the behavior of subsurface NAPL contamination in cold climate regions.

CPP 26.3 Wed 14:30 H39

Invasion Kinetics of Hydrocarbons into Networks of Silica Mesopores — •Simon Gruener[1], Helen E. Hermes[2], Stefan U. Egelhaaf[2], and Patrick Huber[1] — [1]Physics of Mesoscopic Systems, Saarland University, Saarbruecken — [2]Soft Matter Physics, Heinrich-Heine University, Duesseldorf

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 invasion dynamics have been recorded by standard gravimetric measurements, but also by means of neutron radiography experiments. The latter method provides detailed information on the spatial distribution of the liquid within the sample. For one thing this allows for the determination of the liquid's rise height $h(t)$ complementary to the sample's mass increase $m(t)$. Furthermore, insights into the invasion kinetics of the liquid front into the mesoporous network can be gained. Based on these results the occurrence of light scattering at the advancing front can be conclusively traced back to the non-negligible pore size distribution of the applied Vycor glass. This work has been supported within the DFG priority program 1164, Nano- & Microfluidics (Grant No. Hu 850/2).

CPP 26.4 Wed 14:45 H39

Charge transport and diffusion of ionic liquids in nanoporous silica membranes — •Ciprian Iacob, Joshua Sangoro, Sergej Naumov, Rustem Valiullin, Jörg Kärger, and Friedrich Kremer — Institute of Experimental Physics I, University of Leipzig, Linnéstr. 5, 04103, Leipzig, Germany

Charge transport in 1-hexyl-3-methylimidazolium hexafluorophosphate ionic liquid in oxidized nanoporous silicon membranes - prepared by electrochemical etching of (100) p-type silicon- is investigated in a wide frequency and temperature range by a combination of broadband dielectric spectroscopy and pulsed field gradient nuclear magnetic resonance (PFG NMR). By applying the Einstein-Smoluchowski relation to the dielectric spectra, diffusion coefficient is obtained in quantitative agreement with independent PFG NMR measurements. More than 10-fold systematic decrease in the diffusion coefficient from the bulk value is observed in silica nanopores. This is explained within the framework of a model taking into account decreased mobility at the interface of the pore and the nanoporous membrane due to the ability of the hydrogen-bonded ionic liquid to attach to SiO2 surfaces. By that, it becomes possible to probe the size of the adsorption layer and its temperature dependence. This has direct technological implications to the use of ionic liquids in fuel cells and nanobatteries.

CPP 26.5 Wed 15:00 H39

Polymer Flow in Homogeneous and Structured Microchannels — •Raghunath Chelakkot, Roland G. Winkler, and Gerhard Gompper — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

The flow properties of polymers in microfluidic channels are governed by confinement effects and hydrodynamic interactions. We study this interplay by mesoscale hydrodynamic simulations of confined flexible and semiflexible polymers using multiparticle collision dynamics (MPC). The simulations reveal a pronounced bi-directional cross-channel migration, despite the stiffness of the polymer, governed by surface hydrodynamic interactions and anisotropies in the diffusion, respectively. Increasing polymer stiffness enhances surface induced migration. Semiflexible polymers exhibit tumbling dynamics which resembles that of a polymer in shear flow. Simulations of the transport of flexible polymers through a nanopore show that even at weak flow rates the polymers pass through the narrow region of the channel within a finite simulation time. The translocation time distribution for various flow strength has been calculated. Flow induced properties such as asymmetric stretching, relative velocities of the leading and trailing end of the polymers have also been quantified.

CPP 26.6 Wed 15:15 H39

Flow of microliter and submicroliter droplets on inclined surfaces — •David Magerl, Volker Körstgens, and Peter Müller-Buschbaum — TU München, Physik-Department LS E13, James-Franck-Str. 1, 85747 Garching (Germany)

Theory predicts that very small droplets under an external body force show a different behavior than larger drops. The velocity of large drops is dominated by dissipation in the volume, that of small droplets by friction at the substrate. The aim of our work is to find experimental proof to this interesting phenomenon. Therefore we investigate the gravity-driven movement of microliter and submicroliter droplets on inclined surfaces. We measure the velocity of these small droplets as a function of their size. In these experiments both, the surface treatment and the liquid of the droplets have been varied. The experiments are conducted in a saturated atmosphere of the according liquid. First, the droplet size on a horizontally oriented surface is measured by optical means, then the surface is tilted and the velocity of the flowing droplet is determined by the optical investigation of the droplet movement on the incline. We present experiments with toluene and water on silicon surfaces of different surface energies and compare the results to the theoretical simulations.

15 min. break

CPP 26.7 Wed 15:45 H39

The microscopic origin of surface slip: A neutron scattering study of hexadecane at solid interfaces — •Philipp Gutfreund[1,2], Max Wolff[3], Marco Maccarini[2], Stefan Gerth[4], and Hartmut Zabel[1] — [1]Ruhr-University Bochum, 44780 Bochum, Germany — [2]Institut Laue-Langevin, 38042 Grenoble, France — [3]Uppsala University, 75121 Uppsala, Sweden — [4]University Erlangen-Nuernberg, 91058 Erlangen, Germany

A non-sticking contacting layer of a flowing liquid at solid boundaries, called surface slip, is nowadays observed in a wide range of studies exploring microscopic flow. However, the fundamental origin of boundary slip remains unclear. Different mechanisms were proposed like the formation of a thin depletion layer or a molecular ordering in the liquid near the interface, both changing the interfacial velocity profile and, thus, manifesting in apparent slip. Neutron Reflectometry (NR) and Grazing Incident Neutron Diffraction (GIND) are excellent tools for the investigation of buried boundary layers at solid/liquid interfaces in the nm regime. In this contribution we will show a combined NR and GIND study on in situ sheared hexadecane in contact with differently coated solid interfaces. In the case of an attractive interface a depleted layer is observed which is influenced by shear as well as by temperature. For the low interfacial energy substrate no depletion layer is observed. Thus the depletion layer cannot be the origin of surface slip, as for hexadecane slip was observed in both cases.

CPP 26.8 Wed 16:00 H39

Reduced Interfacial Entanglement Density Affects Boundary Condition of Polymer Flow — Oliver Bäumchen[1], •Matthias Lessel[1], Renate Fetzer[1,2], and Karin Jacobs[1] — [1]Saarland University, Experimental Physics, D-66041 Saarbrücken, Germany — [2]Ian Wark Research Institute, University of South Australia, Mawson Lakes, SA 5095, Australia.

Hydrodynamic boundary conditions play a crucial role in the flow dynamics of thin films [1] and can be probed by the analysis of liquid front profiles [2]. For long-chained polymer films it was reported that a deviation from a symmetric profile is a result of viscoelastic effects. In this study [3], however, evidence is given that merely a slip boundary condition at the solid/liquid interface can lead to an asymmetric profile. Variation of molecular weight shows that slippage is directly linked to chain entanglements. We find a reduced entanglement density at the solid/liquid interface (factor 3 to 4), which stresses the importance of considering non-bulk polymer properties in the vicinity of an interface.

[1] O. Bäumchen et al., J.Phys.: Condens. Matter 21 (2009, in press).

[2] O. Bäumchen et al., in IUTAM Symposium on Advances in Micro- and Nanofluidics, edited by M. Ellero, X. Hu, J. Fröhlich, N. Adams (Springer, 2009).

[3] O. Bäumchen et al., Phys. Rev. Lett. (2009, in press).

CPP 26.9 Wed 16:15 H39

The influence of thermal noise and slippage on the dynamics of spinodally dewetting polymer films — •Matthias Lessel, Oliver Bäumchen, and Karin Jacobs — Saarland University, Experimental physics, 66123 Saarbrücken

We investigate the dewetting dynamics of liquid films with thicknesses in the range of a few nanometers. Our experiments focus on spinodally dewetting films [1]. Thermal fluctuations (capillary waves) lead to a variation in film thickness and induce dewetting.

The morphology of the dewetting film can be captured by simulations. Catching the experimental system, the interaction potential, the surface tension and the film thickness are needed [2]. In case of thin polymer films, spinodally dewetting can be monitored in situ by AFM, which reveals the power spectrum of the film thickness variation over time. For the theoretical description, however, experimental viscosity and thermal noise have to be taken into account [3].

Our study now concentrates on the impact of the boundary condition at the liquid/solid interface on the power spectrum. Recently, Rauscher et al. [4] predicted a shift in the power spectrum in case of a slip-boundary condition. To test that prediction, dewetting experiments have been performed on surfaces which provoke strong slippage. First results show the influence of the boundary condition.

[1]:R. Seemann, R. Herminghaus, K. Jacobs, PRL, 86 (2001)

[2]:J. Becker et al., Nat. Mat., 2 (2003)

[3]:R. Fetzer et al., PRL, 99 (2007)

[4]:R. Rauscher et al., Langmuir, 24 (2008)

CPP 26.10 Wed 16:30 H39

Instability of confined water films between elastic surfaces — •Sissi de Beer, Dieter 't Mannetje, Sietske Zantema, and Frieder Mugele — University of Twente, Enschede, the Netherlands

We investigated the dynamics of nanometer thin water films at controlled ambient humidity adsorbed onto two atomically smooth mica sheets upon rapidly approach of the two surfaces into contact. Using a Surface Forces Apparatus (SFA) in the imaging mode, we found that the water films break up into a distribution of small drops with a typical thickness of few nanometers and a characteristic lateral size and spacing of several micrometers. While the characteristic length of the drops is found to be independent of the ambient humidity, the characteristic time of the break-up decreases from ~1s to 0.01s with increasing humidity. The existence, of characteristic length and time scales shows that this break-up is controlled by an instability rather than a * for SFA experiments conventional * nucleation and growth mechanism. These findings cannot be explained by a dispersion-driven instability mechanism like e.g. spinodal dewetting. In contrast, a model incorporating the elastic energies for the deformation of both the mica sheets and the underlying glue layer (i.e. wrinkling) slowed down by the hydrodynamic resistance correctly reproduces the scaling of the characteristic length and time with humidity.

CPP 26.11 Wed 16:45 H39

Advancing and receding contact ancles on structured topographic surfaces — Ciro Semprebon, •Stephan Herminghaus, and Martin Brinkmann — Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany

The static advancing and receding contact angles of a liquid in contact to topographically structured substrate is studied numerically using a minimization of the interfacial energy. As surface topographies we consider a square array of posts with circular or square cross section which is fully characterized by the diameter, spacing, and height of the posts. The materical contact angle of the wetting liquid on the homogeneous surface, θ_o, is varied between 45° and 135°. Depending on the combination of these three parameters, we find transitions between several possible configurations of the liquid-vapor interface as the apparent contact angle θ_a is increased. During this increase the liquid font passes through a sequence of configurations. The instability of the last configuration triggers the detachment from the row of posts and leads to a jump of the contact line to the next row of posts. The resulting advancing contact angle shows a number of unexpected behaviours depending on the materical contact angle and the particular shape of the pillars. For the same systems we determine the corresponding receding angles and the corresponding contact angle hysteresis.

CPP 26.12 Wed 17:00 H39

Dynamics of trapped Brownian particles in shear flows: shear-induced cross-correlations — •Jochen Bammert and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth

Shear flow causes cross-correlations between fluctuations along orthogonal directions of Brownian particle motion. This effect has been measured recently in an experiment [1], where one or two polystyrene beads were trapped by optical tweezers in a specially designed shear flow cell (see also the contribution of A. Ziehl et al.). The results coincide with the predictions of a Langevin model as explained by this contribution and in [2], where the dynamics of a Brownian particle trapped by a harmonic potential and simultaneously exposed either to a linear shear flow or to a plane Poiseuille flow is described. In the shear plane of both flows the probability distribution of the particle becomes anisotropic and takes either an elliptical or a parachute shape or a superposition of both depending on the mean particle position in the shear plane. We have also determined the correlations between two trapped and hydrodynamically interacting particles in a linear shear flow. Again, correlations between orthogonal directions in the shear plane are found, even between different particles.

[1] A. Ziehl, J. Bammert, L. Holzer, C. Wagner, W. Zimmermann, arXiv:0909.0401, to appear in Phys. Rev. Lett.

[2] L. Holzer, J. Bammert, R. Rzehak, W. Zimmermann, arXiv:0911.3264, submitted to Phys. Rev. E

CPP 26.13 Wed 17:15 H39

Dynamics of lipid bilayer formation using water in oil emulsions in microfluidic channels — •Shashi Thutupalli[1], Ralf Seemann[1,2], and Stephan Herminghaus[1] — [1]Max Planck Institute for Dynamics and Self Organization, Göttingen, Germany — [2]Experimental Physics, Saarland University, Saarbrücken, Germany

Using lipid stabilized water-in-oil emulsions, we investigate the process of formation of lipid bilayers between emulsion droplets. For sufficiently high lipid concentrations in the oil phase, the oil-water interface is fully covered by a monolayer of lipid molecules. When two such monolayers are brought together, the oil separating them drains away, thus forming a lipid bilayer. We use a combination of high speed microscopy and electrical measurements to follow the dynamics of oil drainage and the subsequent bilayer formation. We find two typical modes of membrane formation depending on the surfactant concentration: (i) for lower concentrations, a zipper like mechanism where an oil lens rapidly leaves the region between the two lipid monolayers and (ii) at higher concentration the membrane forms as the droplets tend to separate from each other, similar to a decompression effect. In the first case, we find that the oil drainage reaches a typical velocity of 2mm/s, also corroborated by the rise time of the electrical capacitance due to the bilayer. In the latter case, we report on the critical length and time scales of the membrane formation and also the effect of surfactant concentration on the stability of the bilayer formation by decompression.

CPP 27: Poster: Organic Electronics and Photovoltaics

Time: Wednesday 17:30–19:00 Location: Poster C

CPP 27.1 Wed 17:30 Poster C

Charge carrier pair dissociation in polymer:PCBM blends studied using light induced electron spin resonance. — •Tom J. Savenije[1,2], Andreas Sperlich[1], Hannes Kraus[1], Carsten Deibel[1], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]Optoelectronic Materials Section, Department of Chemical Engineering, Delft University of Technology, Julianalaan 136, 2628 BL Delft, The Netherlands — [3]ZAE Bayern, Div. Functional Materials for Energy Technology, D-97074 Würzburg

Blends of conjugated poly alkylsubstituted-thiophenes or thienothiophenes with a soluble fullerene (PCBM) show promising photophysical properties for application as photoactive layers in photovoltaic devices. On excitation of the polymer, fast electron transfer from the donor to the PCBM occurs leading to a charge carrier pair. For efficient charge collection dissociation of this radical pair is required. However, in view of the low dielectric constant of the blend the mechanism of the dissociation process is still unclear. Using light-induced electron spin resonance measurements we show that the geminate radical pair remains in close proximity at temperatures below ca 40 K. At higher temperatures delocalization of the positive charge on the polymer occurs, leading to an effectively larger radical pair distance.

CPP 27.2 Wed 17:30 Poster C

Analysis of solvent residuals in thin films of conducting polymers — •Markus Schindler, Robert Meier, and Peter Müller-Buschbaum — TU München, Physik-Department LS E13, James-Franck-Str. 1, 85747 Garching (Germany)

Since conducting polymers show widespread application possibilities, e.g. in organic solar cells and organic field effect transistors, it is a serious concern to investigate long-time stability and aging. Aging can be enhanced due to remaining solvent embedded in the polymer matrix of thin films. Remaining solvent affects the mobility of the polymers and results in an ongoing change in the microstructure, which is accompanied by changes in the electrical performance.

We investigated the remaining solvent in thin conducting polymer films with neutron reflectivity, utilising the contrast between protonated and deuterated solvents. In addition, we report surface analysis of different polymer blends based on versatile novel conducting polymers using atomic force microscopy. In these films a spatial resolved analysis concerning the solvent content is obtained with STXM measurements.

CPP 27.3 Wed 17:30 Poster C

Determination of intermolecular transfer integrals from DFT calculations — •Björn Baumeier and Denis Andrienko — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Theoretical studies of charge transport in organic conducting systems pose a unique challenge since they require multiscale schemes that combine quantum-chemical, molecular dynamics and kinetic Monte-Carlo calculations. The description of the mobility of electrons and holes in the hopping regime relies on the determination of intermolecular hopping rates in large scale morphologies. Using Marcus theory these rates can be calculated from intermolecular transfer integrals and on-site energies.

Here we present a detailed computational study on the accuracy and efficiency of density-functional theory based approaches to the determination of intermolecular transfer integrals. First, it is demonstrated how these can be obtained from quantum-chemistry calculations by forming the expectation value of a dimer Fock operator with frontier orbitals of two neighboring monomers based on a projective approach. We then consider the prototypical example of one pair out of a larger morphology of Tris(8-hydroxyquinolinato)aluminium (Alq3) and study the influence of computational parameters, e.g. the choice of basis sets, exchange-correlation functional, and convergence criteria, on the calculated transfer integrals. The respective accuracies and efficiencies are compared in order to derive an optimal strategy for future simulations based on the full morphology.

CPP 27.4 Wed 17:30 Poster C

Fabrication of hierarchically ordered crystalline titania thin films — •Martin Niedermeier[1], Gunar Kaune[1], Monika Rawolle[1], Volker Körstgens[1], Matthias Ruderer[1], Jochen S. Gutmann[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department LS E13, James-Franck-Str. 1, D-85747 Garching (Germany) — [2]Max-Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz (Germany)

Thin films of nanostructured titania have received a lot of attention in various applications such as photovoltaics within the last years. Having a well defined morphology is crucial for the functionality and performance of these films because it defines the volume to surface ratio and thereby the surface being available for interface reactions. Increasing the total film thickness is a common approach in order to increase the surface area. The present work focuses on the fabrication of hierarchically structured titania thin films and their crystallinity. A layer-by-layer spin-coating approach is investigated. A solution based sol-gel process using diblock copolymers as a template to obtain nanocomposite films is followed by calcination to obtain crystalline titania structures. The obtained structures are investigated using several imaging techniques like SEM and AFM. The crystallinity and the thickness of the films are analyzed with XRD and XRR.

CPP 27.5 Wed 17:30 Poster C

Controlling the morphology of thin titania films for applications in hybrid solar cells — •Monika Rawolle[1], Matthias A. Ruderer[1], Stefan Prams[1], Qi Zhong[1], Mine Memesa[2], Jochen S. Gutmann[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department LS E13, James-Franck-Str. 1, D-85747 Garching (Germany) — [2]Max-Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz (Germany)

Nanostructured thin films of titania have a variety of applications. For applications in photovoltaics a high absorption coefficient and a large surface area are desirable. A sponge structure is a promising morphology for titania to meet these demands. Block copolymers can be used in a 'good-poor solvent pair' induced phase separation process coupled with sol-gel chemistry to create structured titania films in a reproducible way. We use the amphiphilic diblock copolymer Poly(dimethyl siloxane)-*block*-methyl methacrylate poly(ethylene oxide) [PDMS-*b*-MA(PEO)] as templating agent.[1] Different well defined mixing procedures of sol-gel components (Tetrahydrofuran, 2-Propanol, HCl and titania precursor in addition to the PDMS-*b*-MA(PEO)) of same weight fractions result in small changes in the morphology of the film. The thin films are prepared via spin-coating on silicon substrates. The surface structure is studied with SEM. Information on the morphology in the volume of the film is gained from GISAXS. The layer thickness and structure are studied with XRR, the optical properties with UV/Vis spectroscopy.

[1] G. Kaune et al., ACS Appl. Mater. Interfaces, in press

CPP 27.6 Wed 17:30 Poster C

Performance of organic solar cells with a ferroelectric component — •Krzysztof Kachel, Matthias Richter, Shine Philip, Ioanna Paloumpa, Klaus Mueller, and Dieter Schmeisser — Brandenburgische Technische Universität Cottbus, Angewandte Physik-Sensorik, 03046 Cottbus, Germany

Charge dissociation and recombination are important factors for the efficiency of organic solar cells, even in blended systems of different polymers. As a new approach, the influence of additional blended ferroelectric nanoparticles on the solar cell performance is investigated. The ferroelectric dipole of the nanoparticle causes a local field, which could lead to a longer recombination time of the polaron pairs. As solar cell system we use bulk heterojunction cells or bilayer structures based on regioregular poly(3-hexylthiophene) (P3HT) as the donor and phenyl-C61-butyric acid methyl ester (PCBM) as the acceptor molecule. As ferroelectric additive we use the ferroelectric copolymer poly(vinylidene fluoride trifluoroethylene) (P(VDF-TrFE)) or $BaTiO_3$. The copolymer is spincoated as ultrathin film of 20nm, whereas the $BaTiO_3$ is incorporated as nanodispersion into the donor-acceptor blend. We present the solar cell parameters for the different geometries and ferroelectric materials as a function of ferroelectric content and of the alignment of the ferroelectric dipoles after application of an external electric field.

CPP 27.7 Wed 17:30 Poster C

Spectroscopic investigations of P3HT/PCBM films for organic BHJ solar cells — •Shine Philip, Matthias Richter, Daniel Friedrich, Ioanna Paloumpa, Klaus Mueller, and Dieter Schmeisser — Brandenburg University of Technology Cottbus, Applied Physics and Sensors, K.-Wachsmann-Allee 17, 03046 Cottbus, Germany

Investigations of the electronic structure and composition of regioregular poly(3-hexylthiophene) (P3HT) and phenyl-C_{61}-butyric acid methyl ester (PCBM) based films using Near Edge X-Ray Absorption Fine Structure (NEXAFS) are presented. The measurements were performed at the U49/2-PGM2 beam line of BESSY II, Berlin recording TEY (total electron yield) and TFY (total fluorescence yield) data. Samples prepared by spin coating a mixture of P3HT dissolved in chloroform and PCBM dissolved in chlorobenzene onto ITO (indium tin oxide) coated glass slides were analyzed. Upon measuring the pure P3HT and PCBM, all reported excitations were observed, whereas the blended system is a weighted superposition of the related peaks. Analyzing the data we calculate the composition of the mixture. We also show angular dependent NEXAFS measurements of the P3HT/PCBM blend in order to measure the orientation and distribution of the P3HT polymer. Additionally, we show a new approach for organic solar cell application. $BaTiO_3$ nanoparticles were incorporated as nanodispersion into the donor-acceptor blend or the ferroelectric copolymer poly(vinylidene fluoride trifluoroethylene) (P(VDF-TrFE)) was spincoated as an ultrathin film below the blend.

CPP 27.8 Wed 17:30 Poster C

Preparation and Characterisation of thin Polymeric Films to be used as Gate Dielectrics in Organic Field Effect Transistors — •Jan Hartel, Christopher Keil, and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de

Thin insulating polymer layers are of interest as gate dielectrics for all-organic field effect transistors (OFET). In our structures a DC resistance above 100 GΩ cm was typically reached. In this study, we performed impedance spectroscopy to characterize the dielectric properties of polymer films. A well-defined area of silver was Ar^+-sputter-deposited onto glass. Subsequently different one-component or two-component polymer resins were deposited by spin-coating in a thickness of 6 - 100 μm. These layers were cured according to the respective technical process suggested by the supplier or optimized according to device performance. To complete the measurement structure a second silver layer of equal geometry was deposited on top of the polymer. The dielectric properties of the different films at different preparation conditions and different film thickness were characterized in this capacitor structure. The response to an AC voltage of 0.5 V in the frequency range of 100 Hz to 1 MHz was analyzed to determine the dielectric permittivity. Characteristics expected for an ideal capacitor were obtained for a number of samples and details of the Nyquist plot were compared to commercial capacitors. Samples down to the 5 μm range preserved the dielectric characteristics of bulk samples. The applicability of these films in OFET structures is discussed.

CPP 27.9 Wed 17:30 Poster C

Influence of Packing Motives on Charge Carrier Mobility in Perylene Tetracarboxdiimide Derivatives — •Falk May[1], Valentina Marcon[2], and Denis Andrienko[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Center of Smart Interfaces, Petersenstr. 32, 64287 Darmstadt, Germany

Discotic mesophases are known for their ability to self-assemble into columnar structures and can serve as semiconducting molecular wires. Charge carrier mobility along these wires strongly depends on molecular packing which is controlled by intermolecular interactions.

In this work we compare the influence of side chains on the packing motives of perylene tetracarboxdiimide (PDI) derivatives. Two different (alkyl and glycol) side chains are considered. We first establish how the packing of side chains affects the molecular orientation within the columns using molecular dynamics. Then, using the high temperature non-adiabatic limit of Marcus theory for hopping rates and solving the rate equation for charge transport, we analyze the link between the secondary structure and charge carrier mobility [1]. This analysis eventually provides a pathway to rational design of columnar assemblies of PDI derivatives with high charge mobilities.

[1]V.Marcon et al., J. Am. Chem. Soc., 131, 2009

CPP 27.10 Wed 17:30 Poster C

Crystallization induced phase separation in a double crystalline donor-acceptor diblock copolymer — •Peter Kohn[1], Michael Sommer[2], Mukundan Thelakkat[2], and Thomas Thurn-Albrecht[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany — [2]Angewandte Funktionspolymere, Makromolekulare Chemie I, Universität Bayreuth, 95440 Bayreuth, Germany

A high density of donor-acceptor interfaces ensuring nanoscale domains is of major importance for bulk hetero-junction organic solar cells. Fully functionalized block copolymers consisting of donor- and acceptor-subchains are an attractive class of materials as they inherently carry the desired heterogeneity on the molecular level. We studied the structure formation in a poly(3-hexyl thiophene-b-perylene acrylate) diblock copolymer by temperature dependent small- and wide-angle X-ray scattering. At high temperatures the block copolymer is in the disordered, non-microphase separated state. During cooling separate crystallization of both blocks induces a donor-acceptor phase separation. The resulting morphology of donor- and acceptor crystals separated on the nanoscale demonstrates the potential applicability of this class of materials for organic solar cell devices.

CPP 27.11 Wed 17:30 Poster C

Mobility Measurements of aza-BODIPY for Organic Solar Cells — •Moritz Hein, Roland Gresser, Torben Menke, Karl Leo, and Moritz Riede — Inst. f. Angewandte Photophysik, Dresden, Deutschland

For organic electronics applications, e.g. organic solar cells, new appropriate materials, in particular with high charge carrier mobilities are crucial. This contribution focuses on the promising absorber material class of aza-BODIPY. A series of this new donor material, with four different substituents and increased molecular rigidity has been analyzed in respect of mobility. Depending on the electron donor strength of the substituents, the HOMO (highest occupied molecular orbital) energy of the materials can be tuned from 5.1 eV to 5.7 eV. Structural modification, increasing the rigidity of the molecule and extending the planar pi-conjugated system lead to a better molecular orbital overlap of two adjacent molecules in the crystal structure. We investigate the influence of this structure variation on the mobility. Two different methods are used: field effect transistor (OFET) and space charge limited current (SCLC) measurements. A comparison of the mobilities of the different materials and techniques is presented. Furthermore, the film morphology has a huge influence on the mobility. To study this, the effect of heating the substrate during evaporation is used.

CPP 27.12 Wed 17:30 Poster C

Breakdown of perturbative weak coupling approaches for the biomolecular energy transfer — •Peter Nalbach and Michael Thorwart — Freiburg Institute for Advanced Studies (FRIAS), Albert-Ludwigs-Universität Freiburg, Albertstraße 19, 79104 Freiburg, Germany

We show that the biomolecular exciton dynamics under the influence of slow polarization fluctuations in the solvent cannot be described by approaches which are perturbative in the system-bath coupling. For this, we compare results for the decoherence rate of the exciton dynamics of a resumed perturbation theory with numerically exact real-time path-integral results. We find up to one order in magnitude difference in the decoherence rate for realistically slow solvent environments even in the weak coupling regime, while both results coincide for fast environmental noise. This shows explicitely the nonperturbative influence of the bioenvironmental fluctuations and might render current perturbative approaches to biomolecular exciton transport questionable.

CPP 27.13 Wed 17:30 Poster C

Proton Transport in Self-Assembling Organic Compounds — •Manuel Schrader and Denis Andrienko — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz

Organic phosphonic acid derivatives are promising materials as proton-conducting electrolytes in water-free proton exchange membrane fuel cells. In this work atomistic molecular dynamics simulations of phosphonic-acid functionalized organic conjugated compounds have been carried out. In order to conduct simulations, force fields for these molecules have been developed with the aid of first-principle calculations. In the simulations supramolecular self-assembly in columnar structures and formation of hydrogen bond networks leading to proton transport could be observed.

CPP 27.14 Wed 17:30 Poster C

Imaging the ageing dynamics of polymer solar cells — •Marco Seeland, Rösch Roland, and Hoppe Harald — Institute of Physics, Ilmenau University of Technology, Weimarer Str. 32, 98673 Ilmenau, Germany

Nowadays, many attempts are existing on the route towards higher power conversion efficiencies in polymer solar cells. In addition, the lifetimes of such devices play a key role for the market entry as commercial products. To investigate the timescale of degradation processes, we applied long-time stability measurements with devices stored in the dark and under illumination and compare the results with luminescence images. The application of those techniques allows us to investigate the ageing dynamics in our devices consisting of an interpenetrating network of P3HT and PCBM, sandwiched between the ITO/PEDOT:PSS and aluminium electrode.

CPP 27.15 Wed 17:30 Poster C

Temperature dependent photoinduced absorption measurements on oligothiophene derivatives — •Christian Körner[1], Hannah Ziehlke[1], Karl Leo[1], Roland Fitzner[2], Egon Reinold[2], Peter Bäuerle[2], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden — [2]Institut für Organische Chemie II und Neue Materialien, Universität Ulm

Oligothiophenes are among the most promising small molecules for use in organic photovoltaic devices (OPV). The current efficiency world record of 6.1% on an area of $>2cm^2$ is based on using an oligothiophene derivative as one of the absorber materials. Notwithstanding this success, the underlying processes e.g. for charge generation at the donor-acceptor heterointerface are still subject of intense discussions.

By small variations of the molecule structure we are able to systematically tune the electrical and optical properties of these molecules. The energy levels which are mainly determined by the backbone length and the terminating end groups are supposed to strongly correlate with energy and charge transfer processes like the initial charge separation step at the donor-acceptor heterojunction in OPV.

Here we present temperature dependent PIA measurements of dicyanovinyl end-capped oligothiophenes with various backbone lengths. The nature and recombination dynamics of the long living triplet excitons and cations present in optically excited oligothiophene single layers and in mixed layers with the acceptor C_{60} are determined and compared.

CPP 27.16 Wed 17:30 Poster C

Substituted Perylene Diimides as Electron Acceptors in Organic Solar Cells: Suppressing aggregate and formation to increase device efficiency — •Valentin Kamm, Ian A. Howard, Chen Li, Klaus Müllen, and Frédéric Laquai — Max-Planck-Institut für Polymerforschung, Mainz, Deutschland

Perylene diimide (PDI) is a promising candidate as electron acceptor material for high open circuit voltage organic solar cells. Its strong absorption in the visible region combined with high electron mobility in the solid state renders it a potential alternative to the weakly absorbing PCBM that is typically used in state-of-the-art organic solar cells. However, PDI molecules tend to aggregate and form intermolecular excited states that can act as exciton traps. These traps effectively limit the diffusion of excitons to the interface where charge separation occurs and thus strongly reduce the charge generation efficiency in bulk heterojunction solar cells.

We investigate the effect of different bulky side groups attached to the terminal and to the bay positions of PDI molecules on the formation of aggregates by time-resolved optical spectroscopy. In particular transient photoluminescence and transient absorption spectroscopy are used to study, whether the increased spacing between the PDI molecules, caused by the bulky side groups, can prevent aggregation and intermolecular excited state formation leading to more efficient exciton transport. Furthermore, we correlate the photophysical properties of these materials with the efficiency of bulk heterojunction organic solar cells.

CPP 27.17 Wed 17:30 Poster C

Time-resolved luminescence spectroscopy of biomimetic, self-assembling porphyrins — •Jonas Conradt[1,2], Hendrik Kuhn[1], Peter Marek[3], Manuel Reinhard[2,5], Oliver Lösch[5], Alexander Colsmann[2,5], Uli Lemmer[2,5], Teodor Silviu Balaban[3,4], and Heinz Kalt[1,2] — [1]Karlsruhe Institute of Technology (KIT), Institute for Applied Physics (AP), Karlsruhe, Germany — [2]Karlsruhe Institute of Technology (KIT), Center for Functional Nanostructures (CFN), Karlsruhe, Germany — [3]Karlsruhe Institute of Technology (KIT), Institute for Nanotechnology (INT), Karlsruhe, Germany — [4]Université Paul Cézanne Aix-Marseille III, ISM2 - Chirosciences, Marseille, France — [5]Karlsruhe Institute of Technology (KIT), Institute for Light Technology (LTI), Karlsruhe, Germany

Self-assembling porphyrins represent a promising candidate in order to mimic natural bacteriochlorophylls, the light-harvesting system found in photosynthetic bacteria exhibiting chlorosomes. Such biomimetic porphyrins with a central zinc or magnesium atom show interesting photophysical properties. We performed time-resolved spectroscopy on these porphyrins in order to investigate the properties of monomers as well as self-assembled aggregates. An improved fitting algorithm is developed to identify more reliable the decay-associated spectra and the corresponding decay times. The large extinction coefficient of the porphyrins makes them an interesting candidate for photovoltaic application. They can help to improve the external quantum efficiency of hybrid and dye-sensitized solar cells. Their photovoltaic suitability is investigated.

CPP 27.18 Wed 17:30 Poster C

Morphological degradation of fullerene polymer solar cells — •Vida Turkovic, Chetan Raj Singh, Sebastian Engmann, Maik Bärenklau, Roland Röschi, Gerhard Gobsch, and Harald Hoppe — Ilmenau University of Technology, Weimarer Straße 32, Ilmenau 98693

Typical acceptor materials such as fullerene derivates tend to diffuse and finally agglomerate in blends with polymeric donors, depending on the chemical structure of the donor. This process eventually leads to a morphological destruction of the organic solar cells. The changes in the blend morphology of the thin films accelerate when thermally annealed at increased temperatures. Tapping-mode atomic force microscopy (AFM) measurements provide deeper insight into the nano and micrometer scale of the phase separation observable on the surface of the film. Furthermore, to prove the coarsening of phase separation on various length scales, optical microscopy, UV-Vis, photoluminescence and spectral ellipsometry measurements were conducted. Of special interest is tracking down the formation of fullerene aggregates and correlation of their growth in time.

CPP 27.19 Wed 17:30 Poster C

Influence of electron transport on the efficiency of polymer-based solar cells — •Viktor Kuxhaus[1], Frank Jaiser[1], Dieter Neher[1], and Frank Voges[2] — [1]Institute of Physics and Astronomy, University Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany — [2]Merck KGaA, 64271 Darmstadt, Germany

Recently, we showed that the mobility of electrons in polymer-based solar cells has a large influence on the overall performance of such devices [1]. Here, we investigate the correlation between electron mobility and charge generation effciency in organic bilayer solar cells for a series of electron transporting materials (ETMs) with comparable HOMO and LUMO levels. The electron mobility was measured by transient electroluminescence. Here, a thin M3EH-PPV was used as a sensing layer. The interface between M3EH-PPV and ETM acted as a recombination zone of electrons transported through the ETM layer and holes that are blocked at the interface. Therefore, the electron mobility can easily be determined from the onset of M3EH-PPV emission which is spectrally well separated from the ETM emission. To determine the charge generation efficiency, the different ETMs were combined in bilayer solar cell with PFB as donator.

[1] M. Schubert, R. Steyrleuthner, S. Bange, A. Sellinger, D. Neher, pss(a), DOI: 10.1002/200925312

CPP 27.20 Wed 17:30 Poster C

Organic magnetoresistance effect in unipolar and bipolar devices of conjugated polymers — •Thomas Manicke, Frank Jaiser, Sergey Bagnich, and Dieter Neher — Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Deutschland

For the last few years, several origins of the organic magnetoresistance (OMaR) effect have been discussed. There are three main models to describe this effect, namely the polaron pair, bipolaron and excitonic model. The bipolaron model is mutually exclusive to the other two models and predicts an OMaR effect also for unipolar currents.

We present the results of measurements of the OMaR in unipolar and bipolar devices. Experiments were performed both on a hole-conducting polymer (MEH-PPV) and an electron-conducting polymer (F8BT). We also tested the influence of the cathode material in electron-only devices on the OMaR. The results of these experiments suggest that the bipolaron model is not suited to explain this intriguing effect consistently for all device configurations.

CPP 27.21 Wed 17:30 Poster C

Charge Generation and Recombination in Dye-sensitized Solar Cells — •Michael Meister, Henrike Wonneberger, Chen Li, Klaus Müllen, and Frédéric Laquai — Max-Planck-Institute for Polymer Research, Mainz, Germany

Charge recombination is one of the efficiency limiting processes in bulk heterojunction and dye-sensitized organic solar cells. To determine the presence of charges and the dynamics of charge generation and recombination photoinduced absorption spectroscopy (PIA) and transient absorption spectroscopy (TAS) are particularly useful techniques, since most of the investigated states are non-emissive. These methods allow to investigate all important mechanisms that lead to photocurrent generation beginning with the excitation of the dye, followed by charge transfer to a metal oxide semiconductor and regeneration of the dye by an electrolyte or an organic solid state hole conductor. In this study, we present spectroscopic experiments on dye-doped titanium dioxide films using novel all-organic perylene monoimide dyes as sensitizer with and without solid state hole conductor and on real device structures. We correlate the observed charge generation and recombination dynamics with the device efficiency to understand the relation between dye-structure, photophysics and device performance.

CPP 27.22 Wed 17:30 Poster C

Band bending at interfaces between polymers and electrodes — •Ilja Lange — Universität Potsdam, Institut für Physik und Astronomie, Karl-Liebknecht-Strasse 24/25, 14476 Potsdam-Golm

There is an ongoing discussion on whether bend bending is present in organic semiconductors near metallic contacts and how it affects device properties. Here, we present Kelvin Probe studies on various polymers coated with different thickness on the well known polymeric anode poly(3,4-ethylenedioxythiophene): poly(styrenesulfonate) (PEDOT:PSS). Band bending was detected for poly(3-hexylthiophene) (P3HT), poly{3-hexylthiophene-co-[1,4-(2,2-dithienyl)-5,5-2,3,5,6-tetrafluorbenzene]} (P3HTTFT), poly[2,5-dimethoxy-1,4-phenylene-1,2-ethenylene-2-methoxy-5-(2-ethylhexyloxy)-(1,4-phenylene-1,2-ethenylene)] (M3EH-PPV) and poly[2-methoxy-5-(2'-ethyl-hexyloxy)-1,4-phenylene vinylene] (MEH-PPV). The experimental results can be well fitted with a model that explicitly takes into account a Gaussian density of transport sites [1]. This analysis is based on iterative numerical solution of the carrier density according to Fermi statistics and the one-dimensional Poisson equation. By comparing these results with measurements on films of the same materials on different metals, a consistent picture of bend bending in conjugated polymers is developed.

[1] J.C. Blakesley and N.C. Greenham, J. Appl. Phys. 106, 034507 (2009)

CPP 27.23 Wed 17:30 Poster C

Encapsulation of thin fluorescent polymer films with graphenes — •Philipp Lange[1], Martin Dorn[1], Nikolai Severin[1], David Vanden Bout[2], and Jürgen P. Rabe[1] — [1]Humboldt-Universität zu Berlin, Department of Physics, Newtonstr. 15, 12489 Berlin, Germany — [2]The University of Texas at Austin, Department of Biochemistry and Chemistry, Austin, Texas 78712, USA

Conjugated polymers are widely used as active layers in organic electronics. While they exhibit a high potential for new device concepts and low cost fabrication, they suffer from fast degradation under ambient conditions due to reactions with oxygen and moisture. To achieve reliable and long time operation, commercial organic devices are protected with multilayer encapsulation techniques. Graphene has recently been attracting increasing interest due to its remarkable mechanical, optical and electronic properties, which qualifies it for potential application in future electronic devices. This work addresses the question in how far graphenes deposited on top of a thin organic film can protect it sufficiently from degradation by moisture and oxygen. The polymer films are produced by spincoating on mica after which a graphene layer is deposited by mechanical exfoliation. The degradation of the polymer films is investigated with fluorescence microscopy. Our results indicate a substantial reduction in the degradation of organic material covered by graphene and suggest that graphenes can function simultaneously as transparent electrodes and encapsulation layers in future electronic devices.

CPP 27.24 Wed 17:30 Poster C

Kombination von photothermischer Ablenkungsspektroskopie und Spektralellipsometrie zur Bestimmung der Subbandgap-Absorption in Polymersolarzellen — •Felix Herrmann, Martin Presselt, Roland Rösch, Sebastian Engmann, Maik Bärenklau, Sviatoslav Shokhovets, Harald Hoppe und Gerhard Gobsch — Fachgebiet Experimental Physik I, Institut für Physik & Institut für Micro- und Nanotechnologie, Technische Universität Ilmenau, Weimarer Str. 32, 98693 Ilmenau, Deutschland

In dieser Arbeit wird die photothermische Ablenkungsspektroskopie (PDS) zur Bestimmung des Absorptionskoeffizienten im Subbandgapbereich von verschiedenen Schichten in Polymersolarzellen angewandt.

Die Erwärmung der Probe bei Bestrahlung mit monochromatischem Licht bewirkt eine Verringerung des Brechungsindex des Perfluorhexans, in welchem sich die Probe bei der Messung befindet. Diese Verringerung wird durch die Ablenkung eines He-Ne-Laserstrahls detektiert. Die Methode zeichnet sich durch eine hohe Empfindlichkeit aus.

Die Auswertung des PDS-Signals erfolgt mit Hilfe der aus der Ellipsometrie gewonnenen Schichtdicken und Absorptionskoeffizienten oberhalb der Absorptionskante. Diese Kombination von PDS und Spektralellipsometrie ermöglicht die Bestimmung der Absorptionskoeffizienten verschiedener Schichten von NIR bis UV. In diesem Beitrag werden Ergebnisse für den Subbandgapbereich von P3HT-PCBM bulk heterojunction Solarzellen vorgestellt und diskutiert.

CPP 28: Poster: Biopolymers and Biomaterials

Time: Wednesday 17:30–19:00 Location: Poster C

CPP 28.1 Wed 17:30 Poster C

Knots in viral DNA and proteins: A Monte Carlo test with simplified models — •Daniel Reith[1], Thomas Wüst[2], Peter Cifra[3], Daniel Bölinger[4], and Peter Virnau[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany — [2]The Center for Simulational Physics, The University of Georgia, Athens, GA 30602-2451, USA — [3]Polymer Institute, Slovak Academy of Sciences, 842 36 Bratislava, Slovakia — [4]Max Planck Institute of Neurobiology, 82152 Martinsried, Germany

We investigate the influence of chain stiffness on self-entanglements of a single polymer chain with Monte Carlo simulations. Surprisingly, the number of knotted chains in our equilibrium ensemble increases manifold if a small chain stiffness is imposed and stays large if the stiffness is increased to a point at which the polymer is coiled up inside the capsid. Implications on the internal structure of DNA in viral capsids are discussed. In the second part, we test the influence of sequence on single globular heteropolymers. The entanglements of these states turn out to be very similar to those observed in homopolymers of comparable density. As knots are abundant in globular homopolymers these simulations cannot solve the conundrum why only few knots are observed in globular protein structures[1,2].

[1] P. Virnau, Y. Kantor, and M. Kardar, J. Am. Chem. Soc 127, 15102 (2005).

[2] P. Virnau, L. A. Mirny, and M. Kardar, PLoS Comput. Biol. 2, e122 (2006).

CPP 28.2 Wed 17:30 Poster C

Modification of casein films by rennin enzyme action — •Ronald Gebhardt[1,2], Ulrich Kulozik[1], Christian Riekel[2], Manfred Burghammer[2], and Peter Müller-Buschbaum[3] — [1]TU München, Chair for Food Process Engineering and Dairy Technology, Weihenstephaner Berg 1, 85354 Freising-Weihenstephan, Germany — [2]European Synchrotron Radiation Facility, Grenoble, France — [3]TU München, Physik Department E13, Garching, Germany

The aim of our research is the development of new functional materials on the basis of natural products. As a model system we investigated films of casein micelles whose properties were consciously changed. Beside imaging techniques like AFM, we used grazing incidence small angle X-ray scattering with a micrometer-sized X-ray beam (so called microGISAXS) to investigate the micro- and nanostructure of protein films. The method provides information about the multilevel-structure of casein micelles with high positional accuracy and statistical relevance. We used two different approaches in order to modify the casein film structure by rennin. When added to casein solution prior to film preparation, rennin generated homogeneous particle films by transforming casein micelles into para-casein micelles. Contrary, the coating of casein films by rennin led to a surface near transformation into para-casein-micelles only, while casein micelles inside the film kept their native structures. The latter results will be explained on the basis of a diffusion model (1). (1) R. Gebhardt, M. Burghammer, C. Riekel, U. Kulozik, P. Müller-Buschbaum: Dairy Sci. Technol. (2009) accepted

CPP 28.3 Wed 17:30 Poster C

Mineral Capsules via Mineralization of Emulsions — •Alexander Schulz[1], Bernhard Blümich[2], and Alexander Böker[1] — [1]Lehrstuhl für Makromolekulare Materialien und Oberflächen, DWI an der RWTH Aachen e.V., RWTH Aachen University, Germany — [2]Lehrstuhl für Makromolekulare Chemie, RWTH Aachen University, Germany

Mineral capsules of hydroxyapatite with diameters in the range of 10 to 300 μm are prepared by mineralization of a protein-stabilized oil-in-water emulsion.

An oil-in-water emulsion is prepared via vigorous shaking and stabilized by a protein. Subsequently, the water phase is replaced by a supersaturated solution of calcium and phosphate in water, with citrate as an additive, at a slightly alkaline pH. This solution is exchanged frequently by a fresh supersaturated solution, prepared in the same way. After several days, mineral capsules are obtained. The size varies with the parameters of the preparation, as the structure of the mineral and the number of capsules also do. The analysis of the capsules is performed via SEM-imaging of multiple samples taken at different times of mineralization. The mineral is characterized by EDX-spectra taken from the SEM-samples. Thus, optimum parameters for the mineralization procedure could be identified. Further characterization, like crystal structure and porosity of the material, is carried out by X-Ray diffraction (XRD), electron diffraction and NMR.

CPP 28.4 Wed 17:30 Poster C

Silkworm Silk - A High Pressure SAXS/WAXS Study — •Christina Krywka[1], Igor Krasnov[1], Florian Kunze[1], and Martin Müller[2] — [1]Christian-Albrechts-Universität zu Kiel, Institut für Experimentelle und Angewandte Physik, Leibnizstraße 19, D-24098 Kiel — [2]GKSS Forschungszentrum Geesthacht, Max-Planck-Straße 1, D-21502 Geesthacht

Due to the remarkable mechanical properties of natural silks numerous potential applications exist. However, the nanoscopic structure is still a matter of debate and none of the synthetic silk fibers exhibit mechanical properties comparable to those of the bio-spun fibers.

Degummed silkworm silk (*Bombyx Mori*) is a pure protein fiber consisting only of fibroin. The fiber is a semicrystalline nanocomposite with beta-sheet nanocrystals embedded in a soft amorphous matrix. There is indication for a self-modulation of the fibroin within the silk fiber, leading to a phase-separation between those fibroin residues that can form crystallites and those that can't. If this bimodal nanostructure is a result of a self-arrangement of the different domains of the fibroin molecule, this separation should be able to be disrupted by denaturating conditions, such as high pressure or strong denaturants.

Small and wide-angle X-ray scattering (SAXS and WAXS, resp.) methods with *in situ* high hydrostatic pressure (up to 5 kbar) were employed to investigate the impact of strong denaturants (urea) and undirected stress (pressure) on the crystalline and nanoscopic fiber structure and to gain a clearer view onto the mesoscopic structure of silk fibroin.

CPP 28.5 Wed 17:30 Poster C

Hierarchies in the structural organization of spider silk - A quantitative combined model — •Roxana Ene, Periklis Papadopoulos, and Friedrich Kremer — Institut für Experimentelle Physik I, Leipzig, Germany

Combined time-resolved mechanical and polarized Fourier-transform infrared measurements allow us to determine the interconnection of the nanocrystal and amorphous phases in major ampullate spider silk in the native and supercontracted state [1]. Crystal stress can be measured from the frequency shift of main-chain vibrations. The results show that in both states of silk a serial arrangement between the crystalline and amorphous phase dominates the nanostructure. However, supercontracted silk shows a different behavior before being stretched because a hydrogen-bonded network is formed in the amorphous phase, due to release of pre-stress and hydrophobic effects. A three-component combined model of crystals in serial arrangement with amorphous chains and a fraction of chains bypassing them can describe all states of spider silk, assuming hydrogen bonding of worm-like chains at low pre-strain [2]. Additionally water permeability of dragline silk is studied by measuring changes in amide deuteration [3]. The results show that the chemical exchange of amide hydrogen occurs in a large fraction of amino acids, including b-sheeted alanine residues, suggesting that also the crystalline regions are accessible to water. [1] P. Papadopoulos, R. Ene, I. Weidner, F. Kremer Macromol. Rapid Commun 30, 851-857 (2009). [2] R. Ene, P. Papadopoulos, F. Kremer, Soft Matter 5, 4568-4574 (2009) [3] R.Ene, P. Papadopoulos, F. Kremer (in preparation)

CPP 28.6 Wed 17:30 Poster C

2H NMR Studies on Acylated Transmembrane Fusion Peptides — •Anja Penk[1], Matthias Müller[1], Holger Scheidt[1,2], Dieter Langosch[3], and Daniel Huster[1] — [1]Institut für Medizinische Physik und Biophysik, Universität Leipzig, Leipzig, D — [2]Institut für Biochemie/Biotechnologie, Martin-Luther-Universität Halle-Wittenberg, Halle, D — [3]Lehrstuhl Chemie der Biopolymere, Technische Universität München, Freising, D

Fusion of biological membranes is mediated by integral membrane proteins, often modified by covalent attached hydrocarbon chains. Previously, a series of de novo designed alpha-helical peptides with mixed Leu/Val sequences was presented, mimicking fusogenic transmembrane segments. From this series, we have investigated the peptide LV16 (KKKWL VLVLV LVLVL VLVLV KKK), which was synthesized presenting either a free N-terminus or an N-acylation of 2, 8, 12, or 16 carbons. We used 2H and 31P NMR to investigate the structure and dynamics of these peptide lipid chains in POPC and DLPC bilayers and compared them to the hydrocarbon chains of the surrounding membrane. Except for the C-2 chain, all peptide acyl chains were found to insert well into the membrane. This can be understood from the high local lipid concentration, which the N-terminal lipid chains experience. The insertion of these peptides did not influence the membrane structure and dynamics. Although the longer acyl chains insert into the membrane, there is no length adaptation. In spite of the significantly different lengths of the acyl chains, the fraction of gauche defects in the inserted chains is constant, suggesting similar chain entropies.

CPP 28.7 Wed 17:30 Poster C

Structure and Dynamics of the Myristoyl Lipid Modification of a Src Peptide Determined by 2H Solid-State NMR Spectroscopy — •Holger A. Scheidt[1,2] and Daniel Huster[1] — [1]Institut für Medizinische Physik und Biophysik, Universität Leipzig, Leipzig, Deutschland — [2]Institut für Biochemie/Biotechnologie, Martin-Luther-Universität Halle-Wittenberg, Halle, D

Lipid modifications of proteins are widespread in nature and play an important role in numerous biological processes. The nonreceptor tyrosine kinase Src is equipped with an N-terminal myristoyl chain and a cluster of basic amino acids for the stable membrane association of the protein. We used 2H NMR spectroscopy to investigate the structure and dynamics of the myristoyl chain of myr-Src(2-19) and compare them with the hydrocarbon chains of the surrounding phospholipids in bilayers of varying surface potential and chain length. The myristoyl chain of Src is well inserted in all bilayers investigated. In zwitterionic DMPC membranes, the myristoyl chain of Src is significantly longer and appears 'stiffer' than the phospholipid chains. This is explained by an equilibrium between the attraction due to the insertion of the myristoyl chain and the Born repulsion. In a DMPC/DMPS membrane, where attractive electrostatic interactions come into play, the differences between the peptide and the phospholipid chain lengths are attenuated and the molecular dynamics of all lipid chains is similar. In a much thicker DPPC/DPPS/cholesterol membrane, the length of the myristoyl chain of Src is elongated nearly to its maximum and their order parameters are comparable to those of the surrounding membrane.

CPP 28.8 Wed 17:30 Poster C

Automated solvent artifact removal and base plane correction from multidimensional NMR protein spectra by Auremol-SSA — •Wilhelm Massimiliano Malloni[1], Silvia De Sanctis[1], Elmar W. Lang[1], Klaus-Peter Neidig[2], and Hans Robert Kalbitzer[1] — [1]Institut für Biophysik und physikalische Biochemie, Universität Regensburg, Germany — [2]Bruker Biospin GmbH, Software Abteilung, Germany

Strong solvent signals lead to a disappearance of weak protein signals close to the solvent resonance frequency and to base plane variations all over the spectrum. AUREMOL-SSA method provides an automated approach for solvent artifact removal from multidimensional NMR protein spectra. Its core algorithm is based on singular spectrum analysis (SSA) in the time domain and it is combined with an automated base plane correction in the frequency domain. The SSA technique is an extension of the PCA applied to a time lagged data set that embeds each FID separately in an M-dimensional vector space. The performance of the method has been tested on synthetic and experimental spectra including a two-dimensional NOESY spectrum and a three-dimensional 1H,13C-HCCH-TOCSY spectrum. An extension of the FLATT algorithm for base points selection has been introduced after the solvent removal. Those pure baseline regions are then linearly interpolated and subtracted from the original spectrum. The advantage for practical applications is the complete automation that includes the SSA followed by filtering Fourier transformation, phase correction related to the group delay management and baseline correction.

CPP 28.9 Wed 17:30 Poster C

AUREMOL: Automatic protein structure determination from NMR data — •Harald Donaubauer[1], Tobias Harsch[1], Willhelm Malloni[1], Silivia de Sanctis[1], Bärbel Kieninger[1], Nina Danilova[1], Konrad Brunner[1], Wolfram Gronwald[1], Jochen Trenner[1], Klaus-Peter Neidig[2], and Hans-Robert Kalbitzer[1] — [1]University of Regensburg — [2]Bruker BioSpin

Several approaches to the problem of automated protein structure determination from NMR data exist. The concept for automation is a molecule centred approach where all of the available a priori information is used to eliminate as many free parameters as possible and reduce the amount of information and experimental data. Using a starting structure and as much additional information as possible, like predicted chemical shifts and backbone torsion angles, the assignment and the structure itself are refined in an iterative process. Therefore we are developing AUREMOL, which goal is the reliable and automatic structure determination of biological macro molecules such as proteins from NMR data(1). In AUREMOL included modules are RELAX, which uses complete relaxation formalism to calculate a simulated NOESY NMR spectrum, SIBASA (simulated based sequential assignment), which bases on simulated annealing to determine the chemical shifts of these signals, KNOWNOE, REFINE, which calculates intermolecular distances from a NOESY spectrum and the structure evaluation RFAC. (1)Gronwald, W. and Kalbitzer, H.R. Automated Structure Determination of Proteins by NMR Spectroscopy. 2004, Progr. NMR Spectr. 44, 33-96

CPP 28.10 Wed 17:30 Poster C

Development of an Integrated System for High-Pressure NMR Spectroscopy on Proteins — •Werner Kremer, Markus Beck Erlach, Claudia E. Munte, T. Ernst, Rainer Hartl, M. Arnold, Dörte Rochelt, Dieter Niesner, and Hans Robert Kalbitzer — Institute of Biophysics and Physical Biochemistry, Regensburg

High hydrostatic pressure can induce multiple effects on proteins including denaturation, depolymerization, and changes of side chain protonation state. Pressure induced structural changes can be investigated with high pressure NMR spectroscopy, because different conformers in the energy-landscape of proteins are accessible via their different specific volume. Therefore static pressure in the range from 4-200 MPa has been applied to proteins and peptides. In addition the application of pressure jumps with a microprocessor controlled on-line pressure system has been performed in order to analyze possible structural intermediates which are not accessible by the utilization of static pressure. Quartz, sapphire or ceramic cells are used to handle the proteins in aqueous solutions during the experiment. The best results can be obtained with ceramic cells because they can withstand high pressures and can be easily handled. A completely new autoclave for these ceramic cells has been constructed, including an improved method for pressure transmission, an integrated safety jacket and a fast closing emergency valve.

CPP 28.11 Wed 17:30 Poster C

A NMR Bioreactor Setup for 5 mm High-Resolution Probes at 800 MHz — •Paul Ramm[1,2,3], Werner Kremer[1], Ulrich Bogdahn[2], Ludwig Aigner[3], and Hans Robert Kalbitzer[1] — [1]Department of Biophysics and Biophysical Chemistry, University of Regensburg — [2]Department of Neurology, University of Regensburg — [3]Institute of Molecular Regenerative Medicine, Paracelsus Medical University, Salzburg

NMR spectroscopy (MRS) of cells and tissues provides a quantitative insight into cellular composition and metabolism. A common approach is MRS of cell extracts, which can be used to distinguish e.g. different neural cell types [1]. MRS of living cells more closely resembles the in vivo situation, but is restricted due to unphysiological conditions in a NMR tube. Therefore, we are realizing a cell perfusion setup for a Bruker Avance 800 MHz spectrometer equipped with a 5 mm cryo probe. Immobilized cells can then be perfused with variably composed media saturated with a tunable gas mixture of N_2, O_2, and CO_2. Highly-resolved ^{1}H-NMR spectra (FWHM < 3 Hz) can be acquired with a temporal resolution < 5 min. Based on our former investigations on stem cell-specific biomarkers of neural progenitor cells (NPCs) [2], MRS of NPCs under controllable cell culture conditions will be the next step towards a metabolic profiling and biomarker screening of neurogenesis, leading to both a better understanding of stem cell metabolism and to a possible detection of neurogenesis in humans.

[1] Urenjak J et al., J Neurosci 13 (3), 1993

[2] Ramm P et al., Stem Cells 27 (2), 2009

CPP 28.12 Wed 17:30 Poster C

Xenon-Binding Studies of the Thermophilic Enzyme HisF from Thermotoga maritima Using NMR-Spectroscopy — •Christoph Liebold[1], Felix List[1], Hans Robert Kalbitzer[1], Reinhard Sterner[1], and Eike Brunner[2] — [1]Institute of Biophysics and Physical Biochemistry, University of Regensburg, 93040, Germany — [2]Department of chemistry and food chemistry, Dresden University of Technology, 01062,Germany

The hydrophobic noble gas xenon is known to interact with hydrophobic cavities of macromolecules. Important functional entities of enzymes such as substrate tunnels or the active site often exhibit hydrophobic properties. Therefore, Xe can serve as a probe to explore these entities. [1] Moreover, Xe-binding sites are thought to be centres of increased flexibility, thus providing the possibility of conformational changes required for the function of the enzyme. We evaluated the influence of Xe-binding upon the enzyme HisF from the thermophilic bacterium Thermotoga maritima using ^{1}H-^{15}N HSQC spectra and detected xenon-induced conformational changes mainly for hydrophobic residues located around preexisting cavities within the molecule.This behavior indicates that xenon indeed binds into the aforementioned cavities. Biological implications of our observations are discussed and compared with the results of substrate-binding experiments.

[1] Rubin, S. M.; Spence M. M.; Goodson B. M.; Wemmer D. E. Pines A. Proc. Natl. Acad. Sci. U.S.A, 2000, 97, 9472-9475

CPP 29: Poster: Active Fluids

Time: Wednesday 17:30–19:00 Location: Poster C

CPP 29.1 Wed 17:30 Poster C

Chemotactic predator-prey dynamics — •Ankush Sengupta, Tobias Kruppa, and Hartmut Lowen — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität, Universitätsstrasse 1, D-40225 Düsseldorf, Germany

A discrete chemotactic predator-prey model is proposed in which the prey secrets a diffusing chemical which is sensed by the predator and vice versa. Three different dynamical states are identified which correspond to catching, escaping and steady hunting, and various associated scaling laws are extracted. For the escape process, the predator-prey distance is diffusive for short times but exhibits a transient subdiffusive behaviour which scales as a power law $t^{1/3}$ with time t and ultimately crosses over to diffusion again. The trapping dynamics also shows a scaling of the predator-prey distance with time as $|t - t_{cap}|^{1/3}$, close to the capturing time t_{cap}. We explain these power laws theoretically from the analytic forms of the secreted chemical profiles. This allows us to classify the motility and dynamics of various bacteria and phagocytes.

CPP 29.2 Wed 17:30 Poster C

Interface turbulence in thin liquid films produced by active surfactant — •Sergio Alonso[1] and Alexander S. Mikhailov[2] — [1]Physikalisch-Technische Bundesanstalt, Berlin, Germany — [2]Fritz-Haber-Institut, Berlin, Germany

We consider the case of floating protein machines in a thin liquid film. In this case the propulsion forces are applied to the interface and the asymmetry of the air-water interface produces the alignment of the particles in one direction. By the use of a mesoscopic model for the concentration of the protein machines, we show that the flat interface becomes linearly unstable when the rate of energy supply to the machines exceeds a threshold. Under such conditions an interface turbulence can be observed, characterized by irregular traveling waves and propagating machine clusters. Numerical investigations of this nonlinear regime are performed.

CPP 29.3 Wed 17:30 Poster C

Clockwise-directional circle swimmer moves counter-clockwise in Petri dish- and ring-like confinements — Sven van Teeffelen, •Urs Zimmermann, and Hartmut Löwen — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf, Germany

We consider a self-propelled rod driven by a constant internal force and torque that leads to circular motion in two spatial dimensions and therefore is referred to as a circle swimmer with a characteristic radius given by the torque-to-force ratio. The Brownian dynamics of a circle swimmer in confining Petri dish- or ring-shaped geometry are studied with respect to the mean of the swimmer's position, its steady-state properties and its orientational motion by analytical and computational means. For small torque-to-force ratios, the confinement inverts the orientational sense of the motion: a clockwise-directional circle swimmer moves counter-clockwise in the confinement. Examples for our model include self-propelled colloidal rods, vibrated granular rods and motile bacteria in cylindrical confinements.

CPP 30: Poster: Micro and Nanofluidics

Time: Wednesday 17:30–19:00 Location: Poster C

CPP 30.1 Wed 17:30 Poster C

Limits of DDFT for sheared suspensions — •Markus Rauscher[1,2] and Laura Almenar[1,2] — [1]Max-Planck-Institut für Metallforschung, Stuttgart, Germany — [2]ITAP, Universität Stuttgart, Stuttgart, Germany

Dynamic density functional theory (DDFT) has developed into a versatile tool for modeling the dynamics of interacting Brownian particles. We demonstrate that for the stationary transport of particles advected in straight channel DDFT fails to capture essential features of the system: the density distribution across the channel is changed by the solvent flow, as a result the particle throughput is non-linear in the flow velocity, and the throughputs different particles have to be equal if the particles are so big that they cannot pass each other. We mainly attribute this deficiency of DDFT to the equilibrium approximation for the two-body correlation functions used as a closure relation. And in addition to the grand canonical nature of the density functional.

CPP 30.2 Wed 17:30 Poster C

Evidence for the Absence of the Shear Viscosity Minimum of the Confined Liquid Crystal 8OCB — •Dominik Gerstner, Simon Gruener, and Patrick Huber — Physics of Mesoscopic Systems, Saarland University, Saarbruecken

We present measurements on the capillary rise (spontaneous imbibition) of the lqiuid crystal 8OCB into silica monoliths (porous Vycor) permeated by tortuous pores with radii of 5 nm. The invasion dynamics have been recorded measuring the sample's mass increase $m(t)$ due to the liquid uptake. All obtained curves obey the classical Lucas-Washburn law, thus corroborating bulk-like flow behavior even in such extreme spatial confinement. However, the shear viscosity minimum characteristic of the flow of a nematic liquid crystal is found to be absent. This behavior corroborates the assumption of a paranematic phase beyond the I-N-transition temperature caused by an orientational ordering of the molecules induced by the confining cylindrical pore walls. Optical birefringence measurements on 8OCB in aligned silica nanochannels further support this hypothesis. This work has been supported within the DFG priority program 1164, Nano- & Microfluidics (Grant No. Hu 850/2).

CPP 30.3 Wed 17:30 Poster C

Wetting of hydrophobic periodic nanotemplates on Si-surfaces — •Stefan Wiedemann[1], Stefan Heindl[1], Kay Egloff[2], Alfred Plettl[1], Sabine Hild[3], and Paul Ziemann[1] — [1]Institut für Festkörperphysik, Universität Ulm, 89069 Ulm, Germany — [2]Institut für Experimentelle Physik, Universität Ulm, 89069 Ulm, Germany — [3]Institut für Polymerwissenschaften, Universität Linz, A-4040 Linz, Austria

To influence the wetting behavior of a Si surface, periodically ordered nanomasks were prepared by a micellar[1] and photoseeding technique 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 (<180nm), density (70-500 $1/\mu m^2$) and diameter (10-40nm) of the pillars. After removing the etching mask hydrophobicity of the samples was additionaly modified by coating with HMDS (Hexamethyldisilane), OTMS (Octadecyltrimethoxysilane) or a fluorcarbon-film fabricated by plasma-deposition. Wetting of water was studied by measuring advancing, static and receeding contact angles. First results demonstrate either the Wenzel or Cassie-Baxter-state of water drops on the nanostructured surfaces.

[1] G. Kästle et al., Adv. Funct. Mat. 13, 853 (2003)
[2] A. Seidenstücker et al., submitted
[3] F. Weigl et al., Diamond and rel. Mat. 15 1689 (2006)

CPP 30.4 Wed 17:30 Poster C

Wetting of grooved elastic substrates — •Carsten Herrmann[1], Dominik Michler[1], Konstantina Kostourou[2], Stefan Bommer[1], and Ralf Seemann[1] — [1]Experimental Physics, Saarland University, D-66041 Saarbrücken — [2]MPI for Dynamics and Self-Organisation, Bunsenstraße 10, D-37073 Göttingen

The wetting morphologies on grooved viscoelastic substrates are considered experimentally. Due to their elastic properties, the geometry of rubber substrates is changed in the presence of wetting morphologies by the virtue of the capillary forces. Depending on geometry and wettability of the substrate an attractive or repulsive force between neighboring grooves respectively neighboring ridges emerge. This leads to different wetting scenarios and a lateral ordering of the wetting morphologies. The substrates are fabricated from Polydimethylsiloxane (PDMS) rubber and consist of straight parallel grooves having a rectangular shaped cross section. The wetting morphologies are generated by gas phase deposition and observed in situ by optical microscopy. We explore the lateral order and the shape of the emerging liquid morphologies as function of wettability and geometry.

CPP 30.5 Wed 17:30 Poster C

Visualizing Forced Imbibitions in Porous Media. — •Michael Jung, Kamaljit Singh, and Ralf Seemann — Universität des Saarlandes, Saarbrücken, Germany

As a simple model for forced liquid imbibitions into porous media, we study two-dimensional flow experiments in microfluidic devices, developed from oil-resistant UV-curable glue using a softlithography technique. These devices were first saturated with oil (silicon oils or alkanes). The oil was then displaced by flushing water. We observe the dynamic behavior of liquid front using a CCD camera. The effect of various parameters, such as fluid densities, viscosities, water flow velocities and the size and geometry of the pore space, on the position and the behavior of the liquid front as well as the remaining fraction of trapped oil was investigated in detail.

CPP 30.6 Wed 17:30 Poster C

Wetting of grooved elastic substrates - a theoretical study — •Dominik Michler[1,2], Ralf Seemann[1,2], and Martin Brinkmann[1] — [1]Max Planck Institute for Dynamics and Self-Organization, D-37073 Göttingen — [2]Experimental Physics, Saarland University, D-66123 Saarbrücken, Germany

The wetting of an elastic substrate decorated with a periodic pattern of parallel ridges of rectangular cross section is considered theoretically. A high aspect ratio of the ridges separating two neighbouring grooves allows us to employ Krichhoff's theory for the elastic deformation of thin plates to compute their deformations due to interfacial tension and Laplace pressure. We start our investigation with liquid structures of constant cross section perpendicular to the ridges. On this basis a complete morphology diagram of the liquid can be derived, where the appearance of certain morphologies is given depending on the groove geometry, substrate elasticity, and wettability. Using this quasi-2D approach we first calculate the deformation of the ridges of a single groove filled by liquid. For the case of an array of parallel ridges we predict an ordering of liquid structures in neighbouring grooves. This ordering effect is due to the deformation of the ridges, which leads to changes in the cross section of neighbouring grooves. The theoretical predictions will be compared with experimental results.

CPP 30.7 Wed 17:30 Poster C

Liquid Morphologies in wet granulates with large contact angle — •Marc Schaber[1], Mario Scheel[3], Marco Di Michiel[3], Stephan Herminghaus[2], and Ralf Seemann[1] — [1]Experimental Physics, Saarland University, D-66041 Saarbrücken — [2]MPI for Dynamics and Self-Organisation, Bunsenstraße 10, D-37073 Göttingen — [3]ESRF, 6 rue Jules Horowitz, F-38000 Grenoble

Adding liquid to dry granulates causes the formation of a network of capillary bridges and complex liquid morphologies inside the granulate and typically a stiffening of the granulate is observed. Depending on wettability of the granulate different liquid morphologies are formed. We explore the three dimensional liquid distribution within granulates composed of glass microspheres with a low contact angle and basalt microspheres with a large contact angle using X-ray micro-tomography. The emerging liquid morphologies are analyzed and compared for different liquid contents, contact angles and bead sizes. Using time resolved X-ray tomography we furthermore explore the liquid equilibration process as function of wettability.

CPP 30.8 Wed 17:30 Poster C

Static Wetting Morphologies in Topographically Structured Substrates — •Stefan Bommer[1], Dominik Michler[1], Martin Brinkmann[2], and Ralf Seemann[1] — [1]Saarland University, Experimental Physics,D-66041 Saarbrücken — [2]MPI for Dynamics and Self-Organisation,Bunsenstrasse 10, D-37073 Göttingen

The different wetting morphologies of liquid confined to micron sized trapezoidal grooves are studied experimentally and theoretically. We explore the emerging equilibrium morphologies as function of groove wettability and groove aspect ratio, i.e. the ratio of the groove depth to the groove width. For big aspect ratio the qualitative wetting behavior is expected to be similar to triangular grooves, whereas for decreasing aspect ratio the wetting behavior of rectangular grooves or even individual topographic steps is expected. The grooves are fabricated in silicon by wet etching, whereas the slope of the side walls is given by the crystal lattice of the silicon. The wettability of the substrate is controlled by various self-assembly monolayers and fine tuned with a subsequent oxygen plasma treatment. The wetting morphologies consist of polystyrene deposited from the gas phase and imaged by scanning force microscopy in an intermitted. A morphological diagram is derived analytically by minimizing the surface free energies and using the available software package "Surface Evolver" and compared to the experimental results.

CPP 30.9 Wed 17:30 Poster C

Forced imbibition in porous media using in-situ X-ray microtomography — •Hagen Scholl[1], Marco Di Michiel[2], Kamaljit Singh[1], Mario Scheel[2], Stephan Herminghaus[3], and Ralf Seemann[1] — [1]Saarland University, Experimental Physics, D-

66041 Saarbrücken, Germany — [2]European Synchrotron Radiation Facility, F-38000 Grenoble, France — [3]MPI for Dynamics and Self-Organization, D-37073 Göttingen, Germany

The high energy beamline ID15 at the European Radiation Facility (ESRF) allows acquiring full 3D tomograms with micron scaled spatial resolution in less than 2 s. This time resolution is sufficient for an in-situ insight into the dynamics of driven multiphase flow in porous media. We investigate the motion of a water-oil front advancing into an oil filled granular pile composed of glass or basalt microspheres. We analyse the flow velocity of the aqueous phase, shape of the liquid front, the residual oil saturation on a pore size level. An initially straight liquid front roughens extremely quickly and a dynamic and repeatedly filling and draining of individual pore volumes is observed.

CPP 30.10 Wed 17:30 Poster C

On the shape of surface nanobubbles — Bram Borkent[1], •Sissi de Beer[2], Frieder Mugele[2], and Detlef Lohse[1] — [1]University of Twente, PoF, Enschede, the Netherlands — [2]University of Twente, PCF, Enschede, the Netherlands

In recent years the puzzling appearance of surface nanobubbles on hydrophobic surfaces has attracted a lot of attention. On the one hand, stable Atomic Force Microscope (AFM) imaging of the bubbles should not be possible. Due to the large Laplace-pressure inside these small bubbles, they should dissolve immediately and therefore not exist at all. On the other hand, previous AFM experiments of surface nanobubbles suggested an anomalously large contact angle of the bubbles (i.e. much larger then the macroscopic contact angle) and a possible size dependence. We present precise measurements of the contact angle for nanobubbles of various sizes on smooth highly orientated pyrolytic graphite (HOPG) with cantilevers of different shape, spring constant and surface properties. We find that for all cantilevers the contact angle is constant, within the experimental error, down to of a size 20 nm, and its value is equal to 119o. This result, which is the lowest contact angle for surface nanobubbles found so far, is very reproducible and moreover independent of the cantilever type used, provided that the cantilever is clean and the HOPG surface is smooth. In contrast we find that, for a particular set of cantilevers, the surface can become relatively rough (probably due to precipitated matter from the cantilever onto the substrate). In this case much larger contact angles show up, similar to values reported in literature.

CPP 30.11 Wed 17:30 Poster C

Optimized Droplet Microfluidics for Complex Sol-Gel Reactions — •VENKATACHALAM CHOKKALINGAM[1,2], BORIS WEIDENHOF[3], WILHELM MAIER[3], STEPHAN HERMINGHAUS[2], and RALF SEEMANN[1,2] — [1]Experimental Physics, Saarland University, 66123-Saarbruecken, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Bunsenstr. 10, 37073-Goettingen, Germany — [3]Technical Chemistry Saarland University, 66123-Saarbrücken, Germany

Droplet based microfluidics is used to produce silica particles using a sol-gel synthesis route. The chemicals are stoichiometrically dispensed, mixed, and pre-processed inside a microfluidic device allowing for long operation times without any clogging. Using this approach and optimizing all reaction and processing parameters we generate mesoporous silica particles with a very high surface area of 820 sq.m/g and a narrow pore radius distribution of around 2.4 nm. The sol-gel process developed here for pure silica spheres can easily be modified to produce a large variety of mixed oxides.

CPP 30.12 Wed 17:30 Poster C

Self-Synchronizing Microfludiic Droplets — •Venkatachalam Chokkalingam[1,2], Stephan Herminghaus[2], and Ralf Seemann[1,2] — [1]Experimental Physics, Saarland University, 66123-Saarbruecken, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Bunsenstr. 10, 37073-Goettingen, Germany

An easy to handle device for the synchronized in-situ production of two types of emulsion droplets in a microfluidic device with high dispersed phase volume fraction (up to about 96 %) and excellent monodispersity (variance of the droplet diameter < 1.2 %) is introduced. For this device we combined two single step-emulsification units into one device whereas the droplet production of each individual unit self synchronizes with the other to produce droplets in a strictly alternating way. This double step-emulsification mechanism is very robust and even allows producing two distinct families of droplets with variable size in a fixed number ratio of 1:1 upto 1:4, with each family having identical droplets while maintaining excellent monodispersity (variance always < 1.2 %).

CPP 30.13 Wed 17:30 Poster C

Deriving elastic properties of rubber substrates by analyzing the shape of nanodroplets on their surface — •Konstantina Kostourou[1], Stephan Herminghaus[1], and Ralf Seemann[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, D-37073 Göttingen, Germany — [2]Experimental Physics, Saarland University, 66041 Saarbrücken, Germany

We study the shape of polystyrene (PS) nanodroplets generated by the complete dewetting of a PS thin film on rubber elastic substrates of cross-linked Polydimethylsiloxane (PDMS). We are interested in the full shape of the droplet, i.e. the shape of the air/PS interface, the deformation at the dry side of the three phase contact line (TPCL) and the deformation below the droplet. The exact position of the TPCL is determined by scanning the air/PS interface with Harmonix™ AFM, a tool which allows us to extract the elasticity of the material. Thus, overlapping the topography and elasticity signals, we identify the crossover from PDMS to PS, i.e. the TPCL. In parallel, the deformation at the dry side of the TPCL is compared to the one calculated by existing theories. Using the theoretical model as a fitting function with the Elastic modulus being the only free parameter, we can extract the elasticity of the substrate. Finally, the PS/PDMS interface is also imaged by AFM. Quantifying the deformation below the droplet and applying a nanoindentation model, we can extract the substrate Elastic modulus, which is compared and found in very good agreement with the one calculated by the fitting of the dry side of the TPCL.

CPP 30.14 Wed 17:30 Poster C

Micro-rheology on polymer-grafted colloids — •Christof Gutsche[1], Matthias Krüger[2], Markus Rauscher[3], Rudolf Weeber[4], Jens Harting[4], Yong Woon Kim[5], Roland R. Netz[6], and Friedrich Kremer[1] — [1]Institute of Experimental Physics I, Leipzig University, Germany — [2]Fachbereich Physik, Universität Konstanz, Germany — [3]Max-Planck-Institut für Metallforschung, Stuttgart, Germany — [4]Institut für Computerphysik, Universität Stuttgart, Germany — [5]School of Physics, Korea Institute for Advanced Study, Korea — [6]Physics Department, Technical University Munich, Germany

Optical Tweezers are ideal tools to carry out microfluidic and microrheological experiments with micrometer-sized objects. They enable one to measure without any mechanical contact forces acting on a particle with the extraordinary resolution of up to 5 fN. Experiments are presented on (i) the interaction between two single colloids in media of varying ionic strength [1], (ii) the flow resistance of one blank colloid in a polymer solution [2] and (iii) the flow resistance of single DNA-grafted colloids in different media [3,4].

[1] C. Gutsche et al. Phys. Rev. E 76, 031403 (2007) [2] C. Gutsche et al. J. Chem. Phys. 129, 084902 (2008) [3] C. Gutsche et al. Microfluidic Nanofluidic 2(5), 381 (2006) [4] Y.W. Kim et al. Macromolecules 42, 3650 (2009)

CPP 30.15 Wed 17:30 Poster C

Hydrodynamic effects between rotating objects and chains grafted at a wall — •Steffen Schreiber[1], Thomas Tischer[2], and Walter Zimmermann[1] — [1]Theoretische Physik I, Universität Bayreuth, D-95440 Bayreuth, Germany — [2]Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth, Germany

We investigate two asymmetric, rotating and hydrodynamically interacting dumbbells. When the dumbbells have different asymmetries they rotate asynchronously in an external field. The angle between the dumbbell axes oscillates around a non-vanishing mean value. So the symmetry with respect to time reversal is broken. Depending on the dumbbells' shapes this causes either attraction or repulsion between them as we show in selected phase diagrams.

Secondly we investigate the motion of an ensemble of paramagnetic beads in a rotating magnetic field. After aligning the beads in a linear chain by a static magnetic field we rotate the field. Depending on its rotation frequency and on the field strength we find two regimes: For high rotation frequencies and for low field strengths the ensemble of beads forms spiral structures, whereas for low rotation frequencies and high field strengths the chain breaks up into smaller chains.

Furthermore we examine the hydrodynamic interaction between a semiflexible bead-spring chain and a plane no-slip wall, to which the chain is attached. The chain is exposed to different flow profiles. We find that the hydrodynamic interactions between the chain and the wall cause the chain to bend towards the wall. In oscillating flow fields we find an interesting asymmetric motion of the chain.

CPP 30.16 Wed 17:30 Poster C

Slip length of thin polymer films on substrates with different hydrophobic layers — •Mischa Klos, Matthias Lessel, and Karin Jacobs — Saarland University, Experimental Physics, D-66123 Saarbrücken

The typical volume-to-surface fraction in fluid channels of modern microfluidics is getting smaller and smaller, so the solid/liquid interface becomes more and more important. In classic hydrodynamics, the velocity of a liquid at a channel wall is zero. Yet, a non-zero velocity at the interface could greatly enhance the throughput. This phenomenon is known as 'slippage' with the slip length characterizing its strength. For polymer melts, slippage can be achieved by a hydrophobic coating on, e.g., a Si wafer. The slip length can be inferred from the profile of the liquid front during dewetting of the film. We show the impact of different hydrophobic coatings on silicon substrates on the slip length. As coatings we use an amorphous Teflon (AF1600) layer and silanes with different chain lengths. The Teflon induces nearly no slip whereas the silanes (Octadecyltrichlorosilane (OTS), Dodecyltrichlorosilane (DTS)) provoke slip lengths in the range of micrometers (OTS) to tens of micrometers (DTS). The open question is why a difference between 12 (DTS) and 18 (OTS) carbon atoms on the backbone of the silane molecule can be responsible for the different slip lengths. To answer this question we investigate the dewetting on Hexadecyltrichlorosilane (HTS) with 16 carbon atoms on the back bone.

CPP 31: Poster: Polymer Dynamics

Time: Wednesday 17:30–19:00 Location: Poster C

CPP 31.1 Wed 17:30 Poster C

Semidilute Polymer Solutions under Shear Flow — •Chien-Cheng Huang, Roland G. Winkler, and Gerhard Gompper — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

In shear flow, polymers exhibit remarkably large conformational fluctuations due to tumbling motion, i.e., a polymer stretches and recoils in the coarse of time. In the average, a polymer is aligned, which implies shear thinning at sufficiently large shear rates. To characterize the conformational, dynamical, and rheological properties of semidilute polymers solutions under shear flow, we performed novel mesoscale hydrodynamic simulations combining molecular dynamics simulations and the multiparticle collision dynamics (MPC) approach. At equilibrium, the dependence of the radius of gyration and the zero-shear viscosity on the polymer concentration is in agreement with scaling predictions. The alignment, shear viscosity, and tumbling time are determined for various concentrations and shear rates. In the dilute limit, these quantities are functions of the Weissenberg number only and are in agreement with available analytical theories. Above the overlap concentration, additional density effects are obtained, which cannot be accounted for by the Weissenberg number.

CPP 31.2 Wed 17:30 Poster C

Dynamics of Diblock Copolymers in patterned thin films — •Marianne Heckmann[1], Marcus Müller[2], and Barbara Drossel[1] — [1]Institut für Festkörperphysik, TU Darmstadt — [2]Institut für Theoretische Physik, Georg-August-Universität Göttingen

We investigate the ordering process of symmetric diblock copolymers which are confined between two hard walls. One of the walls has a stripe pattern with stripes that attract the A-component of the copolymer while the opposite wall is neutral. We use dynamic self-consistent field theory in order to describe the ordering of the melt. We are interested in the time until the system is perfectly ordered into perpendicular oriented lamellae and the structures which occur during the ordering process. We present results for different distances between the stripes at the walls in a two-dimensional system for systems with two or three stripes.

CPP 31.3 Wed 17:30 Poster C

Viscoelastic rheology of Polymer dispersed Liquid Crystals — •Marcel Roth[1], Chris Grigoriadis[2], Doris Vollmer[1], George Floudas[2], and Günter K. Auernhammer[1] — [1]Max Planck Institute for Polymer Research, Polymer Physics, 55128 Mainz, Germany — [2]University of Ioannina, Department of Physics, 45110 Ioannina, Greece

Polymer dispersed liquid crystals consist of nematic liquid crystalline droplets embedded in a polymer matrix. Applications as optical diodes are manifold and also include curved modules.[1] A thorough understanding of the mechanical properties of theses devices is essential.

For composites of linear PMMA and 4 cyano-4'-biphenyl (5CB) phase separation is induced by cooling through the isotropic-nematic transition. This process is accompanied by a change from a viscous fluid into an elastic network. We employed rheometry and dielectric spectroscopy (DS) to follow the PMMA and 5CB dynamics, respectively. In rheology, all data could be reduced to a single master curve via time-temperature-superposition, irrespective of initial mixing ratios. This behavior relies on two facts: Firstly, 5CB acts as a plastifier for PMMA and thusly speed up the polymer segmental dynamics. Secondly, the phase separation strictly follows the equilibrium PMMA-5CB phase diagram. DS on the other hand, probes mainly the 5CB dynamics and revealed that a part of 5CB molecules does not crystallize in the presence of PMMA. The speed-up of the dynamics of these molecules is in accord with the restricted rotational diffusion model.

[1] D. Coates, J. Mater. Chem., 1995, 5, 2063 - 2072

CPP 31.4 Wed 17:30 Poster C

Probing macroscopic viscosity on a sub-nm scale in polymers — •Markus Selmke, Subhasis Adhikari, and Frank Cichos — Universität Leipzig, Exp. Physik I, mona

Well known are the results from hydrodynamics for the viscous drag spheres experience upon translation and rotation in a continuous medium. For each mode of Brownian motion in the respective degrees of freedom a diffusion equation may be setup with the well established diffusional parameters of the Stokes-Einstein Relation (SER) and the Debye-Stokes-Einstein Relation (DSER). Our recent results show for the first time that these relations accurately predict the measured rotational diffusion time constants of sub-nm sized single fluorescent probe molecules in the complex environment of a glass-forming polymer (PMA) close to its glass transition temperature. Dielectric spectroscopy however does not and shows a different temperature dependence of relaxation times. Simulations of log-normal distributed time-traces of time-constants which describe normal rotational diffusion explain the observed distributions of relaxation parameters that are used to fit the individual molecules' dynamics. No spatial heterogeneity needs to be assumed, the system seems ergodic. The Synthesis of dual-labeled bola-polymers will enable the probing of this spatially homogeneous but dynamically heterogeneos system in more detail. First results from the synthesis are promising. An extension of the far-field two-point microrheology to near-field nano-rheology has been devised in theory and will give access to both the complex shear modulus as well as insight into hydrodynamics on nm length scales.

CPP 31.5 Wed 17:30 Poster C

Stimuli Responsive Polymer Carpets — •Ihsan Amin[1], Marin Steenackers[2], Ning Zhang[2], André Beyer[1], Rainer Jordan[2,3], and Armin Gölzhäuser[1] — [1]Physik supramolekularer Systeme, Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany — [2]Wacker Lehrstuhl für Makromolekulare Chemie, Technische Universität München, Lichtenbergstrasse 4, 85747 Garching, Germany — [3]Professur für Makromolekulare Chemie, Department Chemie, TU Dresden, Zellescher Weg 19, 01069 Dresden, Germany

We developed an innovative strategy to fabricate freestanding polymeric membranes. An experimentally very easy method has been employed, by combining nanosheets and self-initiated photografting and photopolymerization (SIPGP). The composite films consist of a 1 nm thin crosslinked monolayer of biphenylthiol providing outstanding mechanical properties to the layer on which a soft and stimuli responsive 10-300 nm thick polymer brush layer is grafted, forming so-called polymer carpets. These polymer carpets exhibit remarkable properties (optical, wetting) combining extreme thinness, mechanical stability, robustness, flexibility and unprecedented chemical sensitivity. The membrane thickness as well as its mechanical and chemical properties can be tuned precisely by varying the monomer and polymerization time. Moreover, polymer carpet layers buckle and unbuckle reversibly by applying an external (chemical) stimulus. This unprecedented reversible and fast conformational change is visible with the naked eye and could be applied for the development of new and advanced sensors, displays and micromechanical systems.

CPP 31.6 Wed 17:30 Poster C

single molecule study on heterogeneous dynamics of polymer PMA close to glass transition temperature — •subhasis adhikari, markus selmke, and frank cichos — Molecular Nanophotonics, 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 essentially two pictures of spatial and dynamic heterogeneities.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 by analyzing the rotational diffusion of PDI dye molecule in glassy polymer PMA at both,the ensemble and the single molecule (SM) level close to Tg.From our SM measurements in vacuum in the temperature range (Tg+13K to Tg+22K) we obtain a broad distribution of rotational relaxation times of different individual molecules at a given temperature and the rotational correlation function of a single molecule is well fitted by a stretched exponential decay.The mean of the relaxation time distribution fits perfectly the temperature dependent shear viscosity data.A wealth of new information on the heterogeneous dynamics and structure is further expected from an extension of two point michrorheology to SM optical studies based on fluorescence resonance energy transfer(FRET).We have therefore synthesized bi-labeled(Alexa488 & Alexa546) polystyrene polymer and have been characterized by absorption and emission spectra.First SM FRET measurements are reported.

CPP 31.7 Wed 17:30 Poster C

Permeation of a polymer chain through nanopores – timescales and mechanism — •Sara Marleen Hellenkamp, Andreas Heuer, and Monika Schönhoff — Institute of Physical Chemistry, University of Münster, Corrensstr. 28/30, 48149 Münster, Germany

We investigate the permeation of polymers through the nanoporous wall of hollow capsules, in particular the correlation between polymer molecular weight and exchange time. In a previously analysed system consisting of polyelectrolyte multilayer capsules and poly(ethylene glycol) as probe molecules two scaling regimes were identified [1]. In a theoretical study, a scaling law was derived and confirmed by Monte Carlo simulations, where the polymer is represented as a Rouse chain [2].

In the present study, we combine experiments of chain permeation by diffusion time dependent Pulsed Field Gradient NMR diffusion studies with Monte Carlo Simulation of a polymer chain threaded through a nanopore. The simulations are a first step to understand the whole mechanism of polymer permeation through a nanopore. We investigate the correlation between the exchange time and several parameters, in particularly the chain length and the wall thickness. The final goal of this study is to identify general laws governing chain permeation.

[1] R. Choudhury, P. Galvosas, M. Schönhoff, J. Phys. Chem. (2008)

[2] J. L. A. Dubbeldam, A. Milchev, V.G. Rostiashvili, T.A. Vilgis, Cond. Mat. (2007)

CPP 31.8 Wed 17:30 Poster C

Monte Carlo Study of Semiflexible Star-Branched Polymers in Good Solvents — •Ganna Berezovska and Alexander Blumen — Theoretical Polymer Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

We study the influence of the excluded volume on the local properties of regular semiflexible 3- and 4-arm star polymers in a good solvent, by performing simulations in the framework of the bond fluctuation model. Stiffness is introduced through a bending potential between successive bond vectors and we focus in our investigation on the bond vector correlation functions. In agreement with the partially stretched, freely rotating chain arms model proposed by Guenza et al.[1] the stiffness of the arms becomes larger when approaching the core, but the influence of the core and the correlations between the arms decrease with increasing chain stiffness. Within the same arm the bond vectors show long range correlations which obey power law decays.

[1] M. Guenza, M. Mormino, A. Perico, Macromolecules, 24, 6168, (1991).

CPP 31.9 Wed 17:30 Poster C

Force-induced conformational changes in single polymer chain — •Alexander Gerstmayr, Masoud Amirkhani, and Othmar Marti — Institute of Experimental Physics, Ulm University

During the last decade, conformational properties of macromolecules and its response to an external stimulation have received many attention from various disciplines of scientists. In this work an external stimulation is applied to a single chain of polymer and in-situ atomic force microscopy (AFM) is performed to study the conformational change of the polymer's chain. We used different gas environments and an electric field to stimulate conformational change and chain rotation. The polymer's chain has an extended form in the presence of water vapor and a globule form in the presence of ethanol. We applied torque to the polymer's chain by an uniform electric field that causes an orientation of the chain.

CPP 31.10 Wed 17:30 Poster C

Spectral Diffusion Probing Nanoscale Fluctuations — •Stefan Krause, Daniela Täuber, and Christian von Borczyskowski — Center for Nanostructured Materials and Analysis, Chemnitz University of Technology D-09107 Chemnitz, Germany

Since the first single molecule experiments spectral diffusion is known to occur for almost every single emitter. The reason for this photophysical phenomenon can either be related to intrinsic changes of the conformation of a single molecule which is in most cases not rigid but exhibits different states or to changes of the surrounding environment and the resulting reorientation of environmental dipoles. Thus spectral fluctuations can at one hand give insight into the dynamic process of conformational changes and at the other hand probe dynamical processes in condensed matter on the nanometer scale. Here we present results of our investigation on various types of single molecule in different environments such as polymers and on SiO2 surfaces. We use a homebuilt confocal laser scanning microscope and spectroscopy setup to detect spectral dynamics. The extracted data are analysed and interpreted with a model very similar to that used for two dimensional spatial diffusion processes revealing clear correlations between the types of environment and the degree of spectral fluctuations.

CPP 31.11 Wed 17:30 Poster C

Electric Field Induced Alterations of Block Copolymer Domain Spacings — •Christian W. Pester, Heiko G. Schoberth, and Alexander Böker — Lehrstuhl für Makromolekulare Materialien und Oberflächen and DWI an der RWTH

We investigate the effects of direct current electric fields on a concentrated lamellar polystyrene-*b*-polyisoprene (SI) block copolymer system in toluene by using synchrotron small angle X-ray scattering (SAXS). Measurements were performed in a home-built capacitor with parallel gold electrode geometry at the European Synchrotron Radiation Facility (ESRF) in Grenoble, France. As previously shown, electric fields are able to align bulk copolymer morphologies, whereas increasing field strengths lead to both sub-nanometer size variations of SI block copolymer lamellae in the phase separated regime, as well as to alteration of correlation hole scattering lengths in the mixed state. In this work we were able to show, that the sensitivity (ΔL/E) of the SI copolymer chains towards the electric field varies strongly with the temperature of the system, and a shift in the order-disorder transition temperature regime occurs. Furthermore, non-Gaussian behavior of SI-chains in the phase separated regime was discovered, as various field strengths deform the present lamellae to different degrees. Above T_{ODT} Gaussian behavior is adopted, and, due to the lack of morphology based pre-alignment of the polymer chains, their sensitivity towards the electric field increases. In this state chains themselves can be influenced and deformed away from their Gaussian state.

CPP 31.12 Wed 17:30 Poster C

Micromechanics of Thin Films of Elastomeric Polypropylene — •Martin Neumann[1], Mechthild Franke[1], Andreas Schoebel[2], and Robert Magerle[1] — [1]Chemische Physik, TU Chemnitz, D-09107 Chemnitz — [2]WACKER-Lehrstuhl für Makromolekulare Chemie, TU München, D-85747 Garching

We present a micro-tensile testing setup that allows imaging with scanning force microscopy (SFM) the deformations within the microstructure of approximately 1 μm thick polymer films. This allows correlating directly the micromechanical behavior of a polymeric specimen with its macroscopic stress-strain behavior. In elastomeric polypropylene, a semicrystalline polymer with only 12% crystallinity, we image the deformation behavior of individual crystalline lamellae upon straining and relaxation. Our data shows a large variety of phenomena: bending, kink formation and fragmentation of individual lamella, fixed branching angles between lamellae, as well as locally auxetic behavior of certain crystal complexes. The stress-strain behavior is viscoelastic with elastic moduli in the range between 0.2 to 2 MPa and two relaxation time constants of about 10 s and 300 s, similar as measured for macroscopic specimens.

CPP 31.13 Wed 17:30 Poster C

Glassy dynamics in nanometer thin layers of polystyrene — •Emmanuel U. Mapesa[1], Martin Tress[1], Michael Erber[2], Klaus-Jochen Eichhorn[2], Brigitte Voit[2], Anatoli Serghei[3], and Friedrich Kremer[1] — [1]Universität Leipzig, Germany — [2]Leibniz Institut für Polymerforschung, Dresden, Germany — [3]University of Amherst, USA

Glassy dynamics in nanometer (5 nm - 200 nm) thin layers of polystyrene are studied by Broadband Dielectric Spectroscopy and spectroscopic Ellipsometry. For the dielectric measurements *two* types of sample arrangements were applied using either evaporated metal or doped silicon counter electrodes, the latter being accomplished with nanostructured highly insulating silica spacers. In both cases - within the experimental accuracy of +/- 2 K - *no* change in the mean relaxation rate *and* in the width of the relaxation time distribution function is observed. Coinciding results are obtained by the ellipsmetric measurements.

CPP 31.14 Wed 17:30 Poster C

Real and apparent effects on glassy dynamics in thin polymer layers — •Martin Tress[1], Emmanuel U. Mapesa[1], Anatoli Serghei[2], and Friedrich Kremer[1] — [1]Universität Leipzig, Germany — [2]University of Amherst, USA

Numerous studies report changes of glassy dynamics in thin polymer layers. A careful investigation of the preparative factors reveals that remaining solvent can act as plasticizer and annealing in presence of oxygen or water vapour may cause chain breaking and hence chemical degradation. Futhermore physical aging has to be considered. Additionally to these effects on glassy dynamics there is an apparent effect which arises from the fact that the measured net impedance of a sample is influenced by interfacial effects. Analytical and numerical analysis of a simple layer model show that oxide layers at the interfaces of the electrodes can have strong impact on the dielectric net function of the sample, especially in the case of thin films. Based on an analysis of these real and apparent effects it is found that the molecular dynamics in thin polymer layers is *not* altered down to thicknesses of 5 nm.

CPP 31.15 Wed 17:30 Poster C

Group-specific Motion of Single Perylene Bisimide Molecules at Interfaces — •Danny Kowerko[1], Stefan Krause[1], Richard Börner[2], and Christian von Borczyskowski[1] — [1]Center of nanostructured materials and analytics, TU-Chemnitz, 09107 Chemnitz — [2]Institut für Physik, Universität zu Lübeck 23538 Lübeck, Ratzeburger Allee 160

The motion of single organic molecules is often used as probe for the dynamics in heterogeneous media like polymers. Therefore rotational and conformational fluctuations are analysed with single molecules spectroscopy techniques, providing information on the mobility of the local environment of the molecule. Restricted mobility of the molecule itself can be enforced by functional groups. Here we demonstrate on a single molecule level how perylene bisimide molecular (conformational and rotational) dynamics are changed upon adsorption to SiO2 or quartz glass surfaces. A recently developed multi-parameter single molecule detection set-up allowing for rapid parallel determination of 3-D orientation, spectrum and lifetime is used to demonstrate (pyridyl) group-specific adsorption of PBI to the surfaces and how this fact restricts conformation and orientation dynamics.

CPP 31.16 Wed 17:30 Poster C

Relaxation processes of ABA type block copolymers due to chemical confinement — •Moritz Schwabe and Konrad Samwer — Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

It was shown that block copolymers can have an additional relaxation mode, which is localized in the temperature range between the γ-relaxation and a softening of the system. This mode is discussed as a flipping of new short segments, produced by additional hydrogen bonds (chemical confinement). [1] In this work we systematical determined ABA-block copolymers with dynamic-mechanical analysis to their relaxation modes with a main focus on a chemical confinement due to hydrogen bonds. We could identify three different relaxation modes, whereby two modes seemed to depend on the length of the inner B-block and one of the outer A-blocks. We thank the SFB 602 and the GRK 782 for financial supporting. [1] J. Hachenberg, B. Steisel, U. Nergui, D. Bedorf, M. Buback, K. Samwer, International journal of materials, 2008, 99, 5, 502-506

CPP 31.17 Wed 17:30 Poster C

Dynamics and Morphology of Different Poly(alkylene oxide)s — •Christine Gerstl[1], Gerald Johannes Schneider[1], Jürgen Allgaier[1], Angel Alegria[2], Juan Colmenero[2,3], and Dieter Richter[1] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Centro de Fisica de Materiales, Apartado 1072, 20080 San Sebastian, Spain — [3]Donostia 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 temperature dependent neutron diffraction experiments on four different PAOs with side chain lengths ranging from CH_2CH_3 (poly(butylene oxide)) to $(CH_2)_9CH_3$ (poly(dodecene oxide)). Furthermore, the chain conformation studied by neutron small angle scattering (SANS) will be shown and also compared to literature values of other side chain polymers.

Moreover, the relaxation behaviour of the whole polymer chain as well as the segmental dynamics, which were investigated by means of broadband dielectric spectroscopy and neutron backscattering are presented and compared to theoretical predictions.

CPP 32: Poster: Liquids and Ionic Liquids

Time: Wednesday 17:30–19:00 Location: Poster C

CPP 32.1 Wed 17:30 Poster C

Additivity of the heats of transport in binary liquids — •Steffen Hartmann[1], Gerhard Wittko[1], Werner Köhler[1], Katja Albers[2], Feelly Rüther[2], and Gabriele Sadowski[2] — [1]Physikalisches Institut, Universität Bayreuth — [2]Fakultät Bio- und Chemieingenieurwesen, Universität Dortmund

The coupling between heat and mass transport in multicomponent systems under the presence of a temperature gradient is quantitatively expressed by the Soret coefficient. This coefficient contains true nonequilibrium quantities, the so-called heats of transport, and a thermodynamic factor that can be obtained from equilibrium properties. We have measured the Soret coefficients of a large number of binary mixtures of organic solvents and found an additive model for the heats of transport of equimolar mixtures with a high correlation between predicted and measured values. The necessary thermodynamic factors, which contain the activity coefficients, have been determined from the PC-SAFT equation of state and the group contribution method Modified UNIFAC (Dortmund). Our results show, how the components can be ordered according to their thermophobicity.

CPP 32.2 Wed 17:30 Poster C

Measurement of diffusion and thermal diffusion in ternary mixtures. — •Andreas Königer and Werner Köhler — Physikalisches Institut, Universität Bayreuth

The molecular diffusion process in ternary mixtures is much more complicated than that in binaries, because of additional cross diffusion coefficients.

We have developed a highly sensitive two-color beam deflection technique to measure diffusion and thermal diffusion in ternary fluid mixtures. Simultaneous detection of two laser beams with different wavelengths makes it possible to determine the concentration profile of all three components. By comparing the measured beam deflection signal to a numerical solution of the coupled heat and mass transport equations, the diffusion matrix and the thermal diffusion coefficients can be obtained by a non-linear least squares fitting routine.

We report on first measurements of the Soret-, thermal diffusion, and diffusion coefficients, including cross diffusion, of a mixture consisting of tetralin, dodecane and isobutylbenzene, which are known as reference systems for thermal diffusion in binary mixtures.

CPP 32.3 Wed 17:30 Poster C

Temperature dependent structure of liquid water investigated by means of energy-dispersive X-ray diffraction and molecular dynamic simulations — •Christa Guse, Arnold Simionescu, Benjamin Schünemann, Reinhard Hentschke, and Hartwin Bomsdorf — Fachbereich Mathematik und Naturwissenschaften, Bergische Universität, D-42097 Wuppertal, Germany

X-ray diffraction is investigated in the supercooled region (-10° C to 0° C) and, for comparison, at ambient conditions. By means of an energy-dispersive setup coherent X-ray scatter cross-sections within a wide range of momentum transfer values are monitored simultaneously using relatively simple laboratory equipment. The data are corrected for the energy dependent detector response, geometric broadening effects, sample absorption and Compton-scattering. The corrected diffraction curves are in good agreement with results from the ALS experiment. Additional comparisons with available literature data and with computer simulation results of different rigid water models are presented, relating the scattering intensities to the microscopic H-bond structure and dynamics.

CPP 32.4 Wed 17:30 Poster C

Tracking vapor-liquid coexistence in fluids of charged soft dumbbells — •Heiko Braun and Reinhard Hentschke — Fachbereich Mathematik und Naturwissenschaften
Bergische Universität, 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 Monte Carlo work by Camp and co-workers indicates that a fluid of charged hard dumbbells does exhibit gas-liquid (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. Using the molecular-dynamics technique we present simulation results for the g-l critical point of charged soft dumbbells at fixed dipole moment as function of d. We do find a g-l critical point at finite temperature even at the smallest d value (10^{-4}). Reversible aggregation appears to play less a role than in related model systems as d becomes small. Consequently attempts to interpret the simulation results using either an extension of Flory's lattice theory for polymer systems, which includes reversible assembly of monomers into chains, or the defect model for reversible networks proposed by Tlusty and Safran are not successful. The overall best qualitative interpretation of the critical parameters is obtained by considering the dumbbells as dipoles immersed in a continuum dielectric.

CPP 32.5 Wed 17:30 Poster C

Dipolar particles in an external field: Molecular dynamics simulation and mean field theory — •Ran Jia and Reinhard Hentschke — Fachbereich Mathematik und Naturwissenschaften, Bergische Universität, D-42097 Wuppertal, Germany

Using Molecular Dynamics computer simulation we compute gas–liquid phase coexistence curves for the Stockmayer fluid in an external electric field. We observe a field induced shift of the critical temperature, ΔT_c. The sign of ΔT_c depends on whether the potential or the surface charge density is held constant, assuming that the dielectric material fills the space between capacitor plates. Our own as well as previous literature data for ΔT_c are compared to and interpreted in terms of a simple mean field theory. Despite considerable errors in the simulation results, we find consistency between the simulation results obtained by different groups including our own and the mean field description. The latter ties the sign of ΔT_c to the outside constraints via the electric field dependence of the orientation part of the mean field free energy.

CPP 33: Poster: Charge Effects in Soft and Biological Matter

Time: Wednesday 17:30–19:00 Location: Poster C

CPP 33.1 Wed 17:30 Poster C

A Transport Model for an All Solid State Lithium Ion Battery — Stefan Funken and •Manuel Landstorfer — Institut für Numerische Mathematik, Universität Ulm, Ulm, Germany

New developed solid electrolytes indicate some big advantages for rechargeable lithium ion batteries, e.g. heat and cycling stability. These features yield benefits for cell coupled solar cell/rechargeable battery devices. A priori knowledge of some of the cell parameters is of great interest to eliminate poor material combinations and reduce experimental work.

A continuum mechanical modeling framework at cell level will be presented which takes into account the deintercalation and intercalation of lithium, transport of lithium through the solid electrolyte and electrochemical reactions on the flat phase interfaces. Furthermore the potential drop across the rigid double layer is modeled as Robin boundary condition. The derivation of the transport equation for lithium ion concentration $c_{Li^+}(x,t)$ in the solid electrolyte is done by a free energy functional $F[c_{Li^+}]$ which takes into account repulsive ion-ion interaction. Defining the chemical potential as Frechet derivative of the free energy with respect to concentration, $\mu_{Li^+} = \frac{\delta F[c]}{\delta c}$, and the Flux as $\vec{\Gamma}_{Li^+} = D \cdot \nabla \mu_{Li^+}$ one obtains a diffusion equation with a concentration dependent, non-linear diffusion coefficient.

The full model is a coupled non-linear partial differential equation system which is solved with COMSOL® and own code. Numerical results for discharge behavior of an example cell will be presented.

CPP 33.2 Wed 17:30 Poster C

X-Ray and Neutron Reflectometry Study of Polyelectrolyte Multilayers under Mechanical Stress — •Johannes Früh[1], Adrian Rühm[2], Rumen Krastev[1,3], and Ralf Köhler[1,4] — [1]MPI für Kolloid- und Grenzflächenforschung, Am Mühlenberg 1, 14424 Potsdam, Germany — [2]MPI für Metallforschung, Heisenbergstraße 3, 70569 Stuttgart, Germany — [3]Naturwissenschaftliches und Medizinisches Institut an der Universität Tübingen Markwiesenstraße 55, 72770 Reutlingen, Germany — [4]Helmholtz-Zentrum Berlin, Lise Meitner Campus, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Polyelectrolyte (PE) multilayers (PEM) produced by layer-by-layer (LbL) self assembly technique find application in different fields of the technique. Often the PEM are exposed to mechanical stress which they have to sustain. This makes the studies on mechanical properties of PEM important. Especially interesting is the crossover of internal interactions of PE molecules on molecular level and their mechanical properties as their "macroscopic" representation. Our investigation focuses on the changes of the thicknesses and the roughnesses of thin PEM films when the film is exposed to uniaxial mechanical stress. The PEM were prepared from poly-styrene sulphonate (PSS) and poly-diallyldimethyl-ammonium chloride (PDDA) using LbL technique on sheets of homogeneous and molecularly flat poly-dimethylsiloxane (PDMS) and on glass slides as substrates. A modified reflectometry technique on the substrates was used to investigate the thickness changes of the PEM. The films exhibit ranges of elastic and plastic deformation according to the strength of the applied stress.

CPP 33.3 Wed 17:30 Poster C

Application of Transient Current Measurements at High Voltages to salt containing poly(ethylene oxide) — •Jens Balko, Peter Kohn, Klaus Schröter, and Thomas Thurn-Albrecht — Institute of Physics, Martin-Luther-University Halle-Wittenberg, 06120 Halle, Germany

Poly(ethylene oxide) (PEO) based solid polymer electrolytes attract great interest due to their potential use in battery technology. Though conductivity measurements of salt-polymer complexes are frequently reported the independent determination of the charge carrier density and the mobility of ions is difficult. We studied these two quantities by a recently proposed method using transient current experiments at high voltages. The applicability of this method relies on the complete depletion of ions in the bulk as well as the use of blocking electrodes, i.e. the absence of electrochemical reactions at the metal-polymer interface. At low ion content we find consistent values for the charge carrier density, mobility and conductivity. However at higher lithium salt concentrations electrochemical reactions take place that limit the application of the method. We discuss the influence of salt concentration, electrode material and applied voltage.

CPP 33.4 Wed 17:30 Poster C

Properties of terminally-charged dendrimers with flexible spacer-chains and explicit counterions: A Monte Carlo study — Jaroslaw Klos[1,2] and •Jens-Uwe Sommer[1,3] — [1]Leibniz Institute of Polymer Research Dresden e. V., 01069 Dresden, Germany — [2]Faculty of Physics, A. Mickiewicz University, Umultowska 85, 61-614 Poznan, Poland — [3]Institute for Theoretical Physics, Dresden University of Technology, 01069 Dresden, Germany

We study the properties of terminally-charged dendrimers of generations $G = 5, 6$ with flexible spacers of length $S = 1, 2, 4, 8$ accompanied by explicit counterions in an athermal solvent using Monte Carlo simulations based on the Bond Fluctuation Model. In our study both the full Coulomb potential and the excluded volume interactions are taken into account explicitly with the reduced temperature τ as the main simulation parameter. Our calculations confirm that counterions get localized in the molecules' interior and, in particular, condense on the terminal gropus as τ is lowered. This, in turn, affects the conformational properties of the molecules that weakly swell at intermediate τ due to dominating repulsion between the terminal groups and shrink in the limit of high and low τ, respectively. Like for neutral dendrimers, we find a substantial decrease of monomer densities with the radial distance from the dendrimers' center of mass and backfolding of the terminal groups towards the molecules' interior. Furtheremore, by means of the radius of gyration tensor we conclude that the mean instantaneous shape of dendrimers is spherical for all τ inspected.

CPP 33.5 Wed 17:30 Poster C

The diffusion of charged nanoparticles at the air/water interface — •Tobias Gehring and Thomas Fischer — The University of Bayreuth

We measure the electrostatic effects on the diffusion of nanoparticles at the air/water interface. Using particle tracking of fluorescent nanoparticles on air/water interfaces of different ionic strength we are able to determine the change of diffusion of the particles and hence their immersion into the interface with the salt content. First measurements of those electrostatic effects will be presented.

CPP 33.6 Wed 17:30 Poster C

Dynamics of a tethered polymer chain in an oscillating shear flow: a fluorescence microscopy study — •Maryam Khaksar[1,2], Andre Schroder[1], Thomas Gisler[2], and Carlos Marques[1] — [1]Institut Charles Sadron, rue du Loess Strasbourg Cedex 2 — [2]Universität Konstanz, Fachbereich Physik, D-78457 Konstanz

Advances in fluorescence microscopy of single-molecule DNA and the preparation of well defined surfaces with end-tethered DNA chains has allowed unprecedented scrutiny of the behaviour of single polymer chains near an impenetrable wall in equilibrium as well as out of equilibrium. In this contribution we study the response of single end-tethered DNA molecules to an oscillatory shear flow of frequency ω and shear amplitude γ, using fluorescence microscopy and image processing. At moderate shear amplitude γ the chain behaviour is expected to be controlled by the dimensionless Deborah number $\mathrm{De} = \omega\tau$, where τ is the longest relaxation time of the polymer chain. At low frequencies $\mathrm{De} \ll 1$ a chain can relax faster than the flow cycle and the deformation is expected to be equivalent to the one of a chain in a stationary flow. At large frequencies $\mathrm{De} \gg 1$ the chains cannot relax within an oscillation period and one expects the chains to move coherently with the flow. Using fluorescence microscopy we study the dynamic response of end-tethered λ DNA to the flow in the range $0.1 \ll \mathrm{De} \ll 10$, thus exploring not only the small and large Deborah number regimes but also the full crossover region.

CPP 33.7 Wed 17:30 Poster C

Einfache Herstellung eines Dreischicht Ferroelektrets und Charakterisierung mittels dielektrischer Resonanzspektroskopie — •Lars Holländer, Werner Wirges und Reimund Gerhard — Universität Potsdam, Institut für Physik und Astronomie, Karl-Liebknecht-Str. 24/25, 14476 Potsdam, Deutschland

Ferroelektrete sind sehr nützliche Wandlermaterialien für elektromechanische und elektro-akustische Sensoren und Aktoren. Hier wird ein neues und einfaches Verfahren zur Herstellung piezoelektrisch aktiver Polymerschichtsysteme vorgestellt. Die Mittelschicht ist eine weiche, doppelseitig klebende Folie (3M 468MP), aus der mittels Laserschneiden eine Netzstruktur erstellt wird. Auf diese Mittelschicht werden von beiden Seiten, einseitig metallisierte, kommerziell erhältliche Polykarbonat-Filme (BayerMaterialScience Makrofol DE 6-2) aufgeklebt, wobei sich die metallisierte Seite jeweils außen befindet. Danach werden die Proben mit einer hohen elektrischen Spannung in direktem Kontakt gepolt. Eine Polungsspannung von etwa 4 kV reicht aus, um einen piezoelektrischen d33-Koeffizienten von ca. 150 pC/N (aus der Resonanzkurve bestimmt) zu erhalten. Durch Veränderung der Hohlraumdurchmesser lässt sich die Dickenresonanzfrequenz der Ferroelektrete in einem Bereich von ca. 15 bis 30 kHz variieren. Mit der gleichen Methode lässt sich durch zusätzliches Anlegen einer Gleichspannung das innere elektrische Feld der Probe bestimmen.

Durch das einfache Aufkleben der äußeren Schichten können viele verschiedene Polymer Materialien zur Herstellung der piezoelektrischen Sensoren und Aktoren verwendet werden.

CPP 34: Poster: Elastomers and Gels

Time: Wednesday 17:30–19:00 Location: Poster C

CPP 34.1 Wed 17:30 Poster C

4-arm Star Polymer Networks — •Konrad Schwenke[1,2], Michael Lang[1], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden, Germany — [2]Institute for Theoretical Physics, TU Dresden, 01069 Dresden, Germany

We simulate solutions of 4-arm star polymers with stars of two different types A and B with the help of the Bond Fluctuation Model. We use these solutions to construct networks out of the stars where only types A and B are allowed to react with each other. It is investigated how the properties of the star polymer networks depend on the initial polymer concentration and on the size of the stars. One property that we focus on is the ratio of defects in the network, where we see a strong concentration dependence. This system also serves as a model for networks obtained from non-linear precursors. Our work is motivated by experimental results of Sakai et al [1] who synthesized this novel kind of network which resulted in particular homogeneous model-like network structures.

[1] Sakai et al, Macromolecules 2008 41 (14), 5379-5384

CPP 34.2 Wed 17:30 Poster C

Stress relaxation and viscoelasticity of physically crosslinked networks — •Stephan Baeurle[1], Atsushi Hotta[2], and Andrei Gusev[3] — [1]Institut für Physikalische und Theoretische Chemie, Universität Regensburg, Universitätstr. 31, 93053 Regensburg, Germany — [2]Department of Mechanical Engineering, Keio University, 3-14-1 Hiyoshi Kohoku-ku, Yokohama 223-8522, Japan — [3]Department of Materials, Institute of Polymers, ETH, CH-8093 Zurich, Switzerland

In this presentation we report on a new semi-phenomenological theory, to describe and explain the long-time stress relaxation behavior as well as viscoelasticity of thermoplastic elastomers composed of styrenic-block copolymers. The investigated materials form networks of glassy polystyrene crosslinks, which are physically linked by soft rubbery chain segments made of either polybutadiene or polyisoprene. We demonstrate that the model correctly reproduces the crossover from power-law to stretched-exponential behavior of the stress relaxation at a characteristic crossover temperature, found in recent tensile experiments, and that it provides new insights about the nature of the glassy state in the polystyrene crosslinks.

CPP 34.3 Wed 17:30 Poster C

Predicting water sorption and volume swelling in dense polymer systems via computer simulation — •Henning Hörstermann[1], Reinhard Hentschke[1], Marc Amkreutz[2], Michael Hoffmann[2], and Martin Wirts-Rütters[2] — [1]Bergische Universität Wuppertal, Germany — [2]Fraunhofer-Institut für Fertigungstechnik und Angewandte Materialforschung, Bremen, Germany

Atomistic model structures of amorphous polyamide 6 (PA-6) and of an adhesive system consisting of the diglycidyl ether of bisphenol A (DGEBA) as epoxy resin and isophorone diamine (IPD) as curing agent are generated. In the case of the adhesive, we use a new approach for the generation of the cross-linked polymer networks. This takes into account the chemical reaction kinetics of the curing reaction and thus, results in more realistic network structures. Based on these, the equilibrium water content and the swelling ratio of the DGEBA + IPD networks and the amorphous PA-6 are calculated via computer simulation for different thermodynamic conditions. Therefore, we use a hybrid method combining the molecular dynamics technique with an accelerated test particle insertion method. Our results are in reasonable agreement with experiments and, in the case of the PA-6 system, with results from other computer simulation methods.

CPP 34.4 Wed 17:30 Poster C

Simulating coarse grained filled rubber networks under shear stress — •Fan Zhang, Nils Hojdis, and Reinhard Hentschke — Fachbereich Mathematik und Naturwissenschaften, Bergische Universität, Gauss-Str. 20, 42097 Wuppertal

A simple model for filled rubber networks is studied via stochastic dynamics simulation. The model consists of different types of masses joined via simple short-ranged potentials. One type of mass represents filler particles, whereas a second type represents equivalent rubber volume elements. The filler-filler, rubber-rubber, and filler-rubber interaction potentials may be designed according to the (statistical) mechanical properties of the different interfaces. In this exploratory study the potentials simply are harmonic and merely distinguished by different force constants. A harmonic shear stress is imposed via boundary conditions due to Lees and Edwards. Our results include tan δ vs. temperature for different force constant combinations, shear frequencies, and amplitudes. The mapping of the model onto real materials is discussed.

CPP 34.5 Wed 17:30 Poster C

Electromechanical properties and structural changes of smectic C* liquid crystal elastomers under shear — •Periklis Papadopoulos[1], Patrick Heinze[2], Wilhelm Kossack[1], Friedrich Kremer[1], and Heino Finkelmann[2] — [1]Universität Leipzig, Institut für Experimentelle Physik I — [2]Albert-Ludwigs-Universität Freiburg, Institut für Makromolekulare Chemie

Liquid crystal elastomers combine the electrical and optical properties of liquid crystals with the mechanical ones of polymer networks. In smectic C systems, doping with chiral mesogen induces the formation of domains with permanent electric dipole moment, which exhibit piezoelectric properties. During the simultaneous crosslinking and orientation of the mesogen in a magnetic field a polydomain morphology is obtained, where the piezoelectric effects are averaged out on a macroscopic length scale. The application of shear breaks the symmetry and induces the formation of monodomain structure. In this study the structural changes during stepwise shear are compared with the measurements of the direct piezoelectric effect. It is shown that the piezoelectric coefficient reaches its maximum at a certain shear angle that corresponds to the completion of polydomain to monodomain transformation. The complex coefficient shows a strong dependence on temperature, especially near the smectic to isotropic transition, but also on the static mechanical stress and frequency. The effects are discussed with respect to system non-linearity.

CPP 35: Poster: Glasses and Glass Transition

Time: Wednesday 17:30–19:00 Location: Poster B2

CPP 35.1 Wed 17:30 Poster B2

Glass Transition and Crystallization of n-Alcohols Confined in Silicon Nano-Channels — •René Berwanger, Christoph Schumacher, and Rolf Pelster — FR 7.2 - Experimentalphysik, Universität des Saarlandes, D-66123 Saarbrücken, Germany

We present the investigation of several n-alcohols (C_4H_9OH-$C_{16}H_{33}OH$) in mesoporous silicon and silicon oxide by infrared and dielectric spectroscopy. The temperature of the liquid-solid phase transition and the structure of the solid phase depend on both the chain length and the radius of the pores (r = 3 nm-7 nm).
Long-chain alcohols exhibit a crystalline structure at low temperatures. In confinement this is an orthorhombic β-form, where the molecule axes are perpendicular to the pore axis, while in the bulk state a poly-crystalline structure of orthorhombic β- and monoclinic γ-form is observed[1]. In addition, confinement yields to a lowering of the transition temperatures of the liquid → Rotator-(II)-phase (R_{II}) and $R_{II} \rightarrow$ crystalline phase. On the other hand, short-chain alcohols in narrow pores (r $\approx$ 3nm) form a glassy state at low temperatures, but crystallize in larger pores.

[1] R. Berwanger, A. Henschel, P. Huber, K. Knorr, R. Pelster, Phys. Rev. B, 79, 125442 (2009)

CPP 35.2 Wed 17:30 Poster B2

Structural Relaxation in Disordered Solids Below T_g: Study by Thermal-Cycling Single-Molecule Spectroscopy — Yuri G. Vainer[1], Ivan Yu. Eremchev[1], Andrei V. Naumov[1], and •Lothar Kador[2] — [1]Institute for Spectroscopy, Russian Academy of Sciences, Troitsk, Moscow Reg., 142190, Russia — [2]University of Bayreuth, Institute of Physics and Bayreuther Institut für Makromolekülforschung (BIMF), 95440 Bayreuth, Germany

Structural relaxation processes in disordered solids have been studied between 4.5 K and the glass transition with single-molecule spectroscopy and thermal-cycling experiments. The investigated systems are the amorphous polymer polyisobutylene (PIB) doped with a substituted terrylene (TBT) and the disordered crystal *ortho*-dichlorobenzene (*o*-DCB) doped with terrylene (Tr). Irreversible changes of single-molecule spectra were observed and attributed to relaxation processes in the local environment of the chromophore molecules. The effects of these processes on the individual parameters of low-energy excitations in the glass matrix (two-level systems and quasi-localized low-frequency vibrational modes) were analyzed as a function of temperature for the system TBT/PIB. Surprisingly, a large number of relaxation processes take place far below T_g. The data indicate also that the activation energies of the relaxations are distributed non-uniformly in space.

CPP 35.3 Wed 17:30 Poster B2

Signatures in glassy dynamics of molecular liquids and polymers — •Tilman Schubert, Joshua Sangoro, Ciprian Iacob, and Friedrich Kremer — Institute of Experimental Physics I, University of Leipzig, Linnést. 5, 04103 Leipzig, Germany

Charge transport and glassy dynamics in a variety of amorphous materials are investigatet by Broadband Dielectric Spectroscopy (BDS). Despite the apparently similar Vogel - Fulcher - Tamann - type thermal activation of the characteristic quantities (structural alpha-relaxation rate, diffusion rate and dc conductivity), significant discrepancies are revealed upon application of a model-free derivative technique. Detailed analysis of the dielectric strength and the type of its temperature dependence shows distinct characteristics caused by the differences in the type of molecular interactions involved in the materials studied.

CPP 36: Poster: Nanoparticles and Composite Materials

Time: Wednesday 17:30–19:00 Location: Poster B2

CPP 36.1 Wed 17:30 Poster B2

Dielectric investigation of nanocomposites based on Poly(methyl methacrylate) and Polyhedral Oligomeric Silesquioxanes — •Purv Purohit and Andreas Schönhals — BAM Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12200 Berlin, Germany

Enhancement of polymer properties by use of different types of nanosized fillers is explored continuously from nearly past two decades. Polymer based nanocomposites have shown remarkable improvement in properties as compared to conventional scaled composites because of the length scale of interaction of the nanofillers with the polymer segments. Perseverant efforts are made to fully understand the structure-property relationship of such polymer based nanocomposites. Nanocomposites of Poly(methyl methacrylate) as matrix and MethacrylPOSS (MPOSS) as the nanofiller were prepared. The structure-property relationships of the nanocomposites were analyzed using dielectric spectroscopy. The change in the dynamic glass transition of the polymer with different concentrations of the nanofiller is investigated. Fourier transform infrared spectroscopy and differential scanning calorimetry were used to further investigate the properties of such nanocomposites.

CPP 36.2 Wed 17:30 Poster B2

Conformation and Dynamics of Poly-ethylene-propylene in polymer-silica nano composites — •Klaus Nusser[1,2], Susanne Neueder[1,2], Gerald Johannes Schneider[2], Wim Pyckhout-Hintzen[1], Lutz Willner[1], Aurel Radulescu[2], Vitaly Pipich[2], Olaf Holderer[2], Peter Falus[3], and Dieter Richter[1] — [1]IFF, Forschungszentrum Jülich GmbH, 52425 Jülich — [2]Jülich Centre for Neutron Science at FRM2, 85747 Garching — [3]IN 15, Institute Laue Langevin, 38000 Grenoble

Elastomer filler nano composites are widely used in everyday life. Especially the reinforcement of mechanical properties has been applied for a long time in rubber products. The microscopic mechanisms underlying the macroscopic property changes, however, have not been experimentally clarified yet.

We chose a bottom-up approach to gain more microscopic insight into these mechanisms, starting with a simple model system. The polymer component of the composite material was chosen to be polyethylene-propylene, the filler component silica.

Samples with different volume percent silica in the polymer matrix were investigated by means of Small Angle Neutron Scattering, yielding first insight into the microscopic structure of the polymer chains in the presence of the filler particles. The segmental dynamics was probed by means of Neutron Spin Echo spectroscopy.

CPP 36.3 Wed 17:30 Poster B2

Alignment of Magnetic Nanoparticles in Diblock Copolymer Films under External Magnetic Fields — •Hyeokmin Choe[1], Ezzeldin Metwalli[1], Peter Busch[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department LS E13, James-Franck-Str. 1, 85747 Garching (Germany) — [2]Jülich Centre for Neutron Science at FRM II, Forschungszentrum Jülich GmbH, Lichtenbergstr. 1, 85747 Garching (Germany)

Block copolymers with embedded magnetic nanoparticles have attracted strong interest as a method to fabricate hybrid nanocomposites for wide potential applications in functional devices. Furthermore, controlled assembly of copolymers or hybrids to form aligned or patterned structures is an especially hot topic. Recently, controlled alignment of copolymers or hybrids by magnetic fields is emerging in many aspects, because the non-contacting alignment by magnetic fields is easier to handle and safer than that by electric fields. In this work, we have investigated the alignment of magnetic nanoparticles, which is maghemite, in poly(styrene-b-methylmethacrylate) diblock copolymer films. Films are prepared by solution casting. The external magnetic fields are applied to samples during the casting. We have studied both the influence of different concentrations of magnetic nanoparticles as well as external magnetic fields, and the effect of the different field direction, which means the external fields applied by parallel or perpendicular to the substrate. The structure and morphology of films have been characterized with optical microscopy, atomic force microscopy (AFM), and grazing incidence small angle neutron scattering (GISANS).

CPP 36.4 Wed 17:30 Poster B2

Chain Conformation of Polyethylene-propylene-POSS Nanocomposites — •Andreas Zitzelsberger[1,2], Klaus Nusser[1,2], Gerald Johannes Schneider[2], Wim Pyckhout-Hintzen[1], Lutz Willner[1], Aurel Radulescu[2], Vitaly Pipich[2], and Dieter Richter[1] — [1]IFF, Forschungszentrum Jülich GmbH, 52425 Jülich — [2]Jülich Centre for Neutron Science at FRM2, 85747 Garching

Elastomer-filler composite materials are technically very important and widely used. In particular, the reinforcing effect achieved by the addition of carbon black or silica fillers to a polymer matrix is commonly used to tune macroscopic properties. In contrast to that, plasticizer effects were found recently by adding very small particles. Though its technical significance both effects have not been understood in detail at the microscopic level.

We present recent results of Small Angle Neutron Scattering measurements on the chain conformation of polyethylene-propylene in the presence of nanoparticles (polyhedral oligomeric silsesquioxane) at different temperatures and various filler loadings.

CPP 36.5 Wed 17:30 Poster B2

Conformation and Dynamics of silica-polymer composites — •Gerald J. Schneider[1], Susanne Neueder[1], Klaus Nusser[1], Vitaly Pipich[1], Aurel Radulescu[1], Wim Pyckhout-Hintzen[1], Lutz Willner[1], Bela Farago[2], and Dieter Richter[1] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich — [2]Institute Laue Langevin, Grenoble

Polymer based nano composites play a crucial role in various applications. The unique properties are not only of interest for the classical field of rubber technology. Meanwhile there are several new applications in the area of micro electronics e.g. such as organic batteries. Due to the blending of nano particles and polymers, composites are created which exhibit improved features, e.g. silica-rubber blends show improved tensile properties and silicate plastics are fire retardant. In order to develop new materials with desired features a precise knowledge of the morphology and dynamics at the microscopic length scale is essential. Although a lot of studies exist, up to now the relationship between the properties of nano particles and the macroscopic behavior of the blends, which makes these systems so indispensable for industrial applications, has not been understood.

We present recent results on the structure and dynamics of silica-polymer composites obtained by neutron scattering experiments and compare them with the results of dynamical mechanical measurements.

CPP 36.6 Wed 17:30 Poster B2

Investigation of Assembly formation of quantum dots and dyes on a single molecule particle level in thin liquid films — •Frank Gerlach, Daniela Täuber, Danny Kowerko, and Christian von Borczyskowski — nanoMA, TU-Chemnitz, Institut für Physik

Nanoparticles such as colloidal semiconductor quantum dots (QD) are widely used e.q. as labels in biophysical and medical applications. This has led to quite a number of studies, related to the formation of nanoassemblies formed by QD and dye molecules. The formation of assemblies is a - ligand controlled - sequence of attachments and detachments.

Here we use fluorescence and single molecule methods to explore these dynamics in thin liquid films on silica surfaces. This is a combined study on aggregate formation [1] and diffusion experiments [2].
[1] D. Kowerko, J. Schuster, N. Amecke, M. Abdel-Mottaleb, R. Dobrawa, F. Würthner, C. von Borczyskowski, PhysChemChemPhys, 2009 accepted
[2] D. Täuber, C. von Borczyskowski et al: Diff. Fund. Online Journal 2009 submitted

CPP 36.7 Wed 17:30 Poster B2

Effects of strain and stress amplification in filled polymer melts — •Jan Domurath, Marina Saphiannikova, and Gert Heinrich — Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Strasse 6, 01069 Dresden

When hard filler particles are added to a polymer melt, it is usually assumed that its zero-shear viscosity and therefore the stress increase according to Einstein's or a similar formula. In some papers one finds an alternative approach in which the local strain field is increased according to these formulas. Although both approaches provide the same increase of the shear stress in the linear limit, it is possible that the second approach violates the energy conservation law as the macroscopic and microscopic dissipated energies are not equal anymore. While for the non-linear limit it becomes even less clear whether it is the strain or the stress that is increased by the presence of filler. In this contribution we show that it is necessary to increase both the strain and the stress as originally done by Einstein [1]. As hard filler particles cannot be deformed, the polymer melt experiences a higher microscopic deformation than the macroscopic strain. To satisfy the energy conservation law, the shear stress should also be increased [1, 2]. This combined approach enables us to describe the peculiar behaviour of the overshoot peak observed recently in filled LDPE melts [3].
[1] A. Einstein. Ann. d. Phys. 19, 289 (1906), 34, 591 (1911)
[2] A. Svistkov et al. J. Appl. Mech. Tech. Phys. 50, 493 (2009)
[3] F.R. Costa et al. Adv. Polym. Sci. 210, 101 (2008)

CPP 36.8 Wed 17:30 Poster B2

Precursor loaded PMMA-Colloids: A opportunity to structure arrays of non-closed-packed hexagonally ordered Pt-nanoparticles — •Fabian Enderle[1], Bernd Schüler[1], Alfred Plettl[1], Paul Ziemann[1], Eyk Schreiber[2], Ulrich Ziener[2], and Katharina Landfester[3] — [1]Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm — [2]Institut für Organische Chemie III, Universität Ulm, D-89069 Ulm — [3]MPI für Polymerforschung, D-55128 Mainz

Platinum-precursor loaded colloidal polymethylmethacrylate (PMMA) particles are produced in aqueous solution by a miniemulsion and emulsion technique. The particles were deposited on top of a silicon substrate in a hexagonally ordered monolayer. Such layers were patterned by exposing the colloids to an electron beam or deep ultra violet photons. Then the exposed colloids were removed by a commercial remover. Results on both techniques will be reported and their principal limits discussed. After patterning a monolayer of PMMA spheres, an optimized plasma and annealing step in oxygen is applied to obtain Platinum nanoparticles which still exhibit the original lateral order. The deposited colloids and nanoparticles are analyzed by optical microscope, HRSEM and, due to the electron sensitivity of PMMA, also by AFM. Small precursor loaded PMMA particles show the same behaviour as small Polystyrene particles during the processing [1]. Large precursor loaded PMMA particles behave differently and require further development of the chemical and physical fabrication process.

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

CPP 36.9 Wed 17:30 Poster B2

Pt- and FePt- nanoparticles on the basis of emulsion techniques — •Achim Manzke[1], Stefan Wiedemann[1], Fabian Enderle[1], Alfred Plettl[1], Paul Ziemann[1], Eyk Schreiber[2], Ulrich Ziener[2], Nicolas Vogel[3], Katharina Landfester[3], Johannes Biskupek[4], and Ute Kaiser[4] — [1]Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm — [2]Institut für Organische Chemie III, Universität Ulm, D-89069 Ulm — [3]MPI für Polymerforschung, D-55121 Mainz — [4]Materialwissenschaftliche Elektronenmikroskopie, Universität 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. Different process steps are investigated by HRSEM, HRTEM and XPS giving insight in the plasma- and annealing process and demonstrating e.g. the crystalline structure of the Pt-nanoparticles.

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

CPP 36.10 Wed 17:30 Poster B2

Fluorescence intermittency of single CdSe/ZnS nanocrystals - local probes for silanol groups on silicon oxide — •Cornelius Krasselt[1], Robert Schmidt[1], Jörg Schuster[1,2], and Christian von Borczyskowski[1] — [1]Center for nanostructured materials and analytics nanoMA, TU Chemnitz — [2]now: Fraunhofer-Institute ENAS

Fluorescence intermittency, also known as blinking, appears to be a common feature of many different classes of individual emitters. It is characterized by inverse power law distributions for both the "on" and "off" times [1]. Meanwhile it is generally accepted, that this behaviour is due to trapping and detrapping of charges and correlates with the dielectric properties of the environment surrounding the nanocrystals [2].

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 coated CdSe nanocrystals spincoated on thermally grown silicon oxide. Therefore we have modified the trap density by changing the amount of silanol groups either by annealing or hydroxylation of the silicon oxide. We found atypical distributions for the "on" time statistics which show deviations from the expected power law behaviour only seen at the beginning of the statistics. These deviations depend on the preparation of the silicon oxide and the amount of the silanol groups, allowing a qualitatively correlation between the density of these groups and the blinking of single CdSe/ZnS nanocrystals.

[1] F. Cichos et al.: COCIS 12 (2007), 272
[2] A. Issac et al.: Phys. Rev. B 71 (2005), 161302(R)

CPP 36.11 Wed 17:30 Poster B2

Optical characterization of dye doped silica nanoparticles — •Ines Trenkmann[1], Harald Graaf[1], Sangho Bok[2], Shubhra Gangopadhyay[2], and Christian von Borczyskowski[1] — [1]Chemnitz University of Technology, Institute of Physics, Germany — [2]University of Missouri, Dept. of Electrical and Computer Engineering, USA

Over the last years embedding single dye molecules in a solid state matrix became a matter of interest due to the improved mechanical, thermal and chemical stability. Therefore such hybrids became attractive for various applications such as solid-state dye lasers and chemical sensors [1, 2].

We used various ensemble and single-molecule techniques to analyze the optical properties of organosilicate nanoparticles (3 - 5 nm in diameter), which are marked with the fluorescent dye rhodamine 6G [3, 4]. Besides the fluorescence spectra and lifetime, fluorescence time traces for a large number of single particles were recorded. Thereby the distributions of the on- and off-times follow power-law statistics. Additionally we could observe different sub-groups which differ in the number of observed intensity levels. From this we assumed the average number of embedded dye to 2 - 3 molecules.

[1] García-Revilla, S., et al.: Opt. Mat. 31(2009) 1086]
[2] Wang, H, et al.: J. Phys. Chem. B 102(1998) 7231
[3] Trenkmann, I., et al.: Diffusion Fundamentals submitted
[4] Bok, S. et al.: unpublished results

CPP 36.12 Wed 17:30 Poster B2

Chemical functionalization of carbon nanotubes (CNTs) for preparation of the nanocomposites — •Anastasia Golosova[1,2], Rainer Jordan[2], Joseph Adelsberger[1], Alessandro Sepe[1], Martin Niedermeier[1], Sergio S. Funari[3], Peter Lindner[4], and Christine M. Papadakis[1] — [1]TU München, Physikdepartment E13, Garching — [2]TU München, Department Chemie, Lehrstuhl für Makromolekulare Chemie, Garching — [3]HASYLAB at DESY, Hamburg — [4]ILL, Grenoble, France

CNTs feature a special combination of mechanical, electrical, and thermal properties. In spite of many attempts to obtain CNT/polymer composite materials with extraordinary characteristics, the effective incorporation of CNTs within the surrounding matrix is still challenging. The reason is that, due to effective van der Waals attraction, CNTs form large agglomerates, which behave differently from individual CNTs. Direct chemical modification of CNTs with polymer grafts proved to be efficient to enhance their dispersion ability.

We are using self-initiated photografting polymerization to form stable polymer grafts from vinyl monomers. The procedure was found to be successful for the functionalization of single- and multi-walled CNTs with polystyrene and poly(4-vinylpyridine), which is confirmed by use of Raman spectroscopy and thermo-gravimetric analysis. AFM images show deagglomeration of the CNTs after the modification. SAXS (DESY, HASYLAB) and SANS (ILL, D11) experiments were performed in order to determine the dimensions of the native and modified CNTs and their behavior in solutions.

CPP 36.13 Wed 17:30 Poster B2

Towards Selective Functionalization of Diamonds — •Anke Lämmle, Bernhard Grotz, Rolf Reuter, Fedor Jelezko, and Jörg Wrachtrup — 3. Physikalisches Institut, Universität Stuttgart, Germany

In recent years diamonds have attracted high attention in several fields. Out of many colour centres that can be incorporated in diamond, the nitrogen-vacancy centre (NV) has let in particular nanodiamonds make inroads into such diverse fields like biology [1], magnetometry [2] and single photon plasmonics [3,4]. Using diamonds with NV centres is favorable because it combines an unmatched photostability with chemical inertness, biocompatibility and hardness. However further experiments require a deeper knowledge about surface functionalization and its impact on the NV centre itself. We discuss first steps that might lead to a selective functionalization of diamond surfaces and potential applications.

[1] C.-C. Fu et al, PNAS, 727-732 , Vol. 104, No. 3, 2007
[2] G. Balasubramanian et al, Nature 455, 648-651, 2008
[3] S. Schietinger et al, Nano Letters, Vol. 9, No.4, 1694-1698, 2009
[4] R. Kolesov et al, Nature Physics, Vol. 5, 470-474, 2009

CPP 36.14 Wed 17:30 Poster B2

Analytical and Numerical Studies of End-Modified Polymer Brushes — •Dirk Romeis[1,2] and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e. V., Hohe Strasse 6, 01069 Dresden — [2]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden

We investigate the behavior of grafted polymers, where some of the polymers free ends are modified in size and interaction strength with the surrounding solvent. Recent simulation data [1] revealed remarkable localization effects of these end-groups in densely grafted brushes upon changing the solvent quality, respectively the temperature. Additionally, using the analytical self-consistent field approach for polymer brushes as provided in the limit of strongly stretched chains, we present a model to describe a mixed brush of hydrophobic and hydrophilic polymer chains.
[1] Merlitz, H. et. al. [*Phys.Rev.Lett.* **102**, *115702 (2009)*]

CPP 36.15 Wed 17:30 Poster B2

Preparation and characterization of nanolayered gold-polyelectrolyte composites — •Steffen Mitzscherling, Wolfram Leitenberger, Mareike Kiel, and Matias Bargheer — University of Potsdam, Germany

Composite materials made of gold nanoparticles and polyelectrolyte nanolayers can be prepared by spin-coating or layer-by-layer deposition. We have prepared stratified multilayer-films with a spatial period of 10 nm. The films show very low surface roughness (0.5 nm RMS) and the nanoparticle-layers are well separated by layers containing no gold. These samples were analyzed with X-ray reflectometry, AFM and absorption measurements in the UV-visible range. Bragg-peaks up to the fifth order demonstrate the periodic layering of the sample and AFM shows the packing density of gold particles in the plane. We compare the results obtained by spin-coating and layer-by-layer deposition and discuss the refractive index of the composite material.

CPP 36.16 Wed 17:30 Poster B2

Intaglio Printing of Nanoparticles using Nanostructured Wrinkled Substrates — •Stephanie Hiltl[1], Anne Horn[1], Andreas Fery[2], and Alexander Böker[1] — [1]Lehrstuhl für Makromolekulare Oberflächen und Materialien and DWI an der RWTH Aachen e.V., RWTH Aachen University, D-52056 Aachen, Germany — [2]Lehrstuhl für Physikalische Chemie II, Universität Bayreuth, D-95440 Bayreuth, Germany

In the present project we make use of wrinkled PDMS (Polydimethylsiloxane) substrates to guide the assembly of rod-like TMV (tobacco mosaic viruses) particles. Additionally, an effective method to print the particles from the wrinkles on plain substrates is established.

The nanostructured substrates are produced by oxidizing stretched PDMS with an air plasma, generating a hard oxide top layer. When the PDMS is relaxed the mechanical contrast between the hard top and the elastomeric bottom layer results in sinoidal structured surfaces. In order to assemble the viruses on the wrinkled PDMS surface, we use a simple spin coating technique. Regular virus stripes with variable line spacings are generated over large areas in a lithography free process [1]. Wrinkled substrates with pre-aligned TMV are used as "inked" stamps to transfer the virus on flat substrates. The distance of the virus stripes is determined by the wavelength of the stamp. A small amplitude (few tens of nanometers) is crucial for intaglio printing as the ink (virus) is situated in the grooves of the structure. The residual water film, from spin coating the virus, serves as transfer medium for the particles.

[1] Horn et al., Faraday Discuss., 2009, 143, 143-150

CPP 36.17 Wed 17:30 Poster B2

Time resolved spectroscopy and lifetime measurements of single semiconductor nanocrystals — •Robert Schmidt, Cornelius Krasselt, and Christian von Borczyskowski — TU Chemnitz, Institute of Physics, Department of Optical Spectroscopy and Molecular Physics (OSMP), nanoMA (Center for nanostructured Materials and Analytics)

The photoluminescence of single emitters like semiconductor quantum dots (QDs) shows intermittency, called blinking, which divides the intensity time traces into bright "on"-, dark "off"-and intermediate-states. The distribution of "off"-times shows power law behavior with an exponential decay. While the power law behavior of "off"-times is well understood, it is less evident for "on"-times.

We investigate the blinking-dynamics of CdSe/ZnS-nanocrystals using time resolved confocal microscopy, spectroscopy and lifetime measurements. The intensity time traces are analysed with special focus on intermediate intensities, by varying the threshold separating the on- and off- from intermediate-states. Further the intensity time traces are compared with spectral- and lifetime- time traces in order to obtain correlations between intensities, lifetimes and spectral positions. We will report new insights into the intrinsic dynamics of QD.

CPP 36.18 Wed 17:30 Poster B2

Optical investigations of plasmons generated in silver nanowires and their influence on the emission of dye molecules — •Florian Feil, Melari Davies, Christophe Jung, Angela Wochnik, Christina Scheu, Jens Michaelis, and Christoph Bräuchle — Department für Chemie und Biochemie, Ludwig-Maximilians-Universität München, Butenandtstrasse 11, 81377 München

In recent years there has been a growing interest in coupling of plasmons created in nanostructures such as particles and wires to luminescent particles such as dye molecules or quantum dots. In particular, silver is known for exhibiting plasmon resonances for particle sizes in the nanometer regime. Also the shape of the metal, e.g. the aspect ratio of silver nanowires, has a tremendous influence on the plasmonic properties. Therefore it is first important to characterize the nanowires themselves, because small defects can create local emitting entities. In this work, silver nanowires were synthesized and characterized using transmission electron microscopy (TEM) and fluorescence microscopy. They exhibit interesting fluorescence dynamics such as fluctuations in intensity during laser illumination as well as spectral dynamics. We were able to correlate these effects to the structure of the nanowires by overlaying fluorescence and TEM data. Very interestingly, synchronous emission at several micrometer separated positions of the nanowire could be observed, which requires coupling through the wire. These nanowires were then used to enhance the emission of single fluorescent dye molecules deposited in their vicinity.

CPP 36.19 Wed 17:30 Poster B2

Structure factor of the ferrofluid with chain aggregates: influence of an external magnetic field — •Elena Pyanzina[1], Sofia Kantorovich[1,2], Juan Cerda[2], and Christian Holm[2] — [1]Ural State University, Ekaterinburg, Russia — [2]ICP, University of Stuttgart, Stuttgart, Germany

We analyze the structure factor of a ferrofluid with strong interparticle magnetic dipole-dipole interaction. Results on mono- and bidisperse model systems in the presence 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.

CPP 36.20 Wed 17:30 Poster B2

The influence of particle size distribution on the ground-state structures in ferrofluid monolayers — •Victor Danilov[1], Taisia Prokopieva[1], Sofia Kantorovich[1,2], and Christian Holm[2] — [1]Ural State University, Ekaterinburg, Russia — [2]ICP, University of Stuttgart, Stuttgart, Germany

The study of ground state structures in magnetic fluids is of fundamental interest, as it provides the insight into the complex microstructer of the systems.

The analysis of the microstructure of ferrofluid monolayers at low temperatures with single defect particle, which we have carried out recently, is now extended to the generic bidisperse system. Earlier we showed that a single large defect tends to align ”regular” particles along its magnetic field lines, the critical parameters at which the transition from a single ferroparticle ring into a complex structure occurs were found. The dependence of the system ground state structures on the number and size of numerous defects are studied by using of Monte Carlo simulations technique in combination with analytical approach and compared to the case of a single defect.

CPP 36.21 Wed 17:30 Poster B2

Auger release of a deeply trapped carrier in a quantum dot — •Thomas Hartmann[1], Peter Reineker[1], and Vladimir I. Yudson[2] — [1]Abteilung Theoretische Physik, Universität Ulm, 89069 Ulm — [2]Institute for Spectroscopy, Russian Academy of Sciences, Troitsk, Moscow region, 142190, Russia

For a quantum dot (QD) we have studied the transiton between the dark and the bright states on the basis of an Auger-induced release process of an electron deeply trapped in a QD shell. The importance of this release process mechanism in connection with the dark state termination has not been noticed before. The considered release mechanism originates from an elcectron-hole pair which is created by light irradiation and whose energy - after recombination - is transferred to the trapped electron via a Förster-like mechansism $\sim 1/r_0^6$, where r_0 is the distance between the QD center and the trap in the shell. The spatial distribution of deep traps over the QD results in a distribution of "off-times". For a homogeneous spatial distribution of traps and a Förster-like dependence of the trapping probability, the distribution of the "off-times" follows a power law $\sim 1/t_{\rm off}^{3/2}$ with the exponent 3/2 observed experimentally in many QDs.

CPP 36.22 Wed 17:30 Poster B2

Femtosecond pump-probe spectroscopy of the dielectric function of a polymer matrix with embedded gold nanoparticles — •Mareike Kiel[1,2], Peter Gaal[1], Marc Herzog[1], Wolfram Leitenberger[1], Steffen Mitzscherling[1], Torsten Sievers[2], Helmuth Möhwald[2], and Matias Bargheer[1,2] — [1]Universität Potsdam, 14476 Potsdam — [2]Max-Planck-Institut für Kolloid- und Grenzflächenforschung, 14476 Potsdam

We investigate a multilayered compound system of polyelectrolytes and gold nanoparticles with femtosecond pump-probe spectroscopy. A 530nm pump beam excites the electronic system of the nanoparticles, which triggers a breathing mode by electron-phonon coupling and causes strong changes in the dielectric function of the compound material. Relative changes of transient absorption and reflection spectra are measured simultaneously with light in the visible and near infrared region. From this we directly obtain the changes in the real and imaginary part of the compound's dielectric function. By comparison of measurements at near infrared and visible probe wavelengths and application of analytical models, we can separate the contributions from interband and intraband absorption. We also decompose the static absorption spectra into its scattering, plasmon absorption and interference components.

CPP 36.23 Wed 17:30 Poster B2

Optical Detection of Charged Quantum Dots in Solution — •Nicole Amecke-Mönnighoff and Frank Cichos — Molecular Nanophotonics Group, University of Leipzig, Linnéstraße 5, 04103 Leipzig

The fluorescence properties of semiconductor Quantum Dots (QDs) are intensively studied due to many potential applications, which want to make use of their tunable emission wavelength, high quantum yield and photon statistics. Additionally some peculiarities like power-law blinking, lifetime-fluctuations and spectral diffusion can be found. Most of those can be explained by charges close to or in the dot center leading to Auger processes and the quantum confined stark effect. Charges can arise from ejection of electron or hole via tunneling leaving behind the counterpart. One of the main ideas is, thus, the development of an experimental method and setup for controlling and investigating those charges on the single particle level, while monitoring the particles' flourescence. We thus combine confocal microscopy with a setup of two electrodes in solution. When applying a voltage, we can measure the intensity and lifetime changes of the particles in different distances close to the electrode. What we surprisingly find is electrophoresis of a great part of QDs possessing a net positive charge, even though being dispersed in the non-polar solvent toluene. Furthermore they were still fluorescent and no measurable change in lifetime was detected, which is very interesting to the basic understanding of charges quenching a QDs fluorescence. Our goals now are determining this charge's origin, amount and precise location, including also that of the counter charge.

CPP 37: Poster: Colloids and Complex Liquids

Time: Wednesday 17:30–19:00 Location: Poster B2

CPP 37.1 Wed 17:30 Poster B2

Organization of Colloids in Ferrofluids — •Ayan Ray and Thomas Fischer — Universität Bayreuth, 95440 Bayreuth, Germany

Colloidal particles (magnetic and non-magnetic) are the basic building blocks of complex structures with unique optical properties. When these mono-disperse particles with controlled shape, size, volume, and concentration are dispersed in a ferrofluid in a static magnetic field they self-assemble into symmetric arrangements. Here we try to demonstrate the dynamical behavior of a mixture of paramagnetic and non magnetic colloidal particles in a ferrofluid under the influence of a rotating magnetic field.

CPP 37.2 Wed 17:30 Poster B2

Pearl chain to cluster transition dynamics of paramagnetic colloids in a rotating magnetic field — •Nebojsa Casic and Thomas Fischer — Univesitaet Bayreuth 95440 Bayreuth Germany

In a static magnetic field paramagnetic colloids form pearl chains, while the equilibrium conformation in a rotating field is a two dimensional cluster. When switching from a static to a rotating magnetic field a transient dynamics from a pearl chain to a two-dimensional cluster is observed. Two different dynamical regimes of cluster formation are observed. At low frequencies of the magnetic field the colloidal pearl chains fragment into rotating doublets that reassemble into clusters. At high frequencies each pearl chain curls up into two spirals wrapping the chain into a cluster. Attempts to explain the behavior in both regimes are presented.

CPP 37.3 Wed 17:30 Poster B2

Liquid-gas phase transition in a ferrofluid monolayer in an external field — •Heiko Schmidle and Sabine H.L. Klapp — Technische Universität Berlin, Institut für Theoretische Physik, Hardenbergstr. 36, 10623 Berlin

We present the results of a theoretical study of a ferrofluid monolayer in an external field. Magnetic films attract a great dels of interest in experimental studies and they reveal a variety of interesting structures. In order to model the ferrofluid we use a Stockmayer fluid. The particles interact via a Lennard-Jones potential, combined with a dipole moment. The particles are confined to a plane, whereas the dipoles can rotate in three dimensions. This model represents in an accurate way nanoparticles like colloids that are on an plane. We investigate the influence of an external field on the liquid-gas phase transition. We use extensive Monte-Carlo simulations in the grand canonical ensemble. Long range-interactions are handeled by Ewald summation techniques. Histogram reweighting and preweighted multicanonical simulations are used in order to determine the exact transition curve of the ferrofluid monolayer.

CPP 37.4 Wed 17:30 Poster B2

Pearl chain to cluster transition dynamics of paramagnetic colloids in a rotating magnetic field — •Nebojsa Casic and Thomas Fischer — Universität Bayreuth Bayreuth Germany

Duplicate of poster CPP 37.2.

CPP 37.5 Wed 17:30 Poster B2

2D versus wire-like structures: exploring the deposition conditions for self-assembling polystyrene nanoparticles — ●Matthias Schwartzkopf[1], Mottakin Abul Kashem[1], Adeline Buffet[1], Gerd Herzog[1], Volker Körstgens[2], Peter Müller-Buschbaum[2], Jan Perlich[1], Stephan V. Roth[1], Stephan Förster[3], and Rainer Gehrke[1] — [1]HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg, Germany — [2]Physik-Department E13, TU München, James-Franck-Str. 1, D-85748 Garching, Germany — [3]Universität Hamburg, Institut für Physikalische Chemie, Grindelallee 117, D-20146 Hamburg, Germany

Installing regular arrays on mesoscopic length scales plays an important role in nanoscience. Different techniques of self-assembly via solvent evaporation have been used to obtain highly ordered colloidal structures. We used Langmuir-Blodgett (LB) technique and spray deposition, representing the most attractive tools for the formation of larger homogeneous colloidal arrays. During their different deposition and boundary conditions, the assembly behaviour of polystyrene nanoparticles changes, resulting in two-dimensional layers with LB-technique and stripe-like pattern by spray deposition. We present our first results from atomic force microscopy and microbeam grazing incidence small-angle x-ray scattering.

CPP 37.6 Wed 17:30 Poster B2

Transient melting of binary glasses by hot gold colloids — ●Florian Schwaiger and Werner Köhler — Universität Bayreuth, Physikalisches Institut, 95440 Bayreuth

Gold colloids with a diameter of 250 nm can be heated by laser irradiation and have been used as microscopic heat sources in near-critical polymer blends (poly(ethyl-methyl siloxane)/poly(dimethyl siloxane)) and in concentrated polystyrene/toluene solutions close to the glass transition. Due to the high absorbance at the plasmon resonance wavelength ($\lambda \approx 532$ nm), significant temperature gradients $\nabla T \propto 1/r^2$ can be achieved in the close vicinity of the particles on length scales below the diffraction limit. As a consequence of the Soret effect, there is a strong coupling to the order parameter, the local composition of the binary system. Colloids immobilized at a surface have been used to induce composition patterns in the polymer blend. In the binary glass former, a bubble of high mobility due to local toluene enrichment, accompanied by a lowering of T_g, is formed around and moves together with the colloidal particle.

CPP 37.7 Wed 17:30 Poster B2

A new experimental setup for microscopic studies of confined colloids in quasi-2d — ●Alexander Reinmüller, Thomas Palberg, and Hans Joachim Schöpe — Institut für Physik der Universität Mainz, Staudingerweg 7, D-55099 Mainz, Germany

Both equilibrium and non-equilibrium behaviour of confined many particle systems is of great scientific interest. To investigate confined colloidal model systems we constructed a new experimental high-precision setup. The confinement consisting basically of flat quartz plates can be adjusted precisely by use of special Piezo drives allowing a variable plate to plate distance (contact - 100 micrometers) and the application of compression and shear forces. The experimental setup is designed for observations using common optical scientific microscopes. The goal of our experiments is the investigation of the phase behaviour of mono-disperse and bi-disperse Yukawa systems as well as their non-equilibrium behaviour. We present the new setup as well as first interesting results of fully deionized charged spheres in confinement.

CPP 37.8 Wed 17:30 Poster B2

Colloidal suspensions of magnetic particles in time-dependent external fields — ●Sebastian Jäger — Institut für Theoretische Physik, Technische Universität Berlin

We investigate colloidal suspensions of magnetic particles in 3 dimensions that interact with time-dependent external fields. The particles are modelled by dipolar soft spheres, whose dipolar coupling strength is such that it enables chain and cluster formation even if no external field is present. We choose the coupling of the dipoles with the external field to be even stronger than the dipole-dipole coupling strength. The states under scrutiny include low density dilute states as well as high density fluid states. Our methods include Molecular Dynamics simluations at fixed temperature and Brownian Dynamics simulations. In these simulations, we utilize the Ewald summation method to treat the long-range dipolar interactions.

CPP 37.9 Wed 17:30 Poster B2

Suppression of Multiple Scattering in Colloidal Model Systems — ●Achim Lederer and Hans-Joachim Schoepe — Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Deutschland

Light scattering is one of the most power full tools in soft matter physics to study the structure, kinetics and dynamics of the system of interest. Unfortunately the evaluation of conventional light scattering data is often complicated due to multiple scattering effects. In colloidal model systems multiple scattering can often be suppressed in particle form factor measurements by dilution or index matching methods, whereas it is a difficult task determining the structure factor. By a new designed Two Colour Dynamic Light Scattering setup, multiple scattering free dynamic and static light scattering data are obtained and compared to other multiple scattering free methods.

CPP 37.10 Wed 17:30 Poster B2

Optical Tweezers to Measure the Interaction Forces between Poly(2-vinylpyridine) Brushes — ●Mahdy M. Elmahdy[1,3], Alla Synytska[2], Astrid Drechsler[2], Christof Gutsche[1], Petra Uhlmann[2], Manfred Stamm[2], and Friedrich Kremer[1] — [1]Institute of Experimental Physics I, Leipzig University, Linnéstrasse 5, 04103, Leipzig, Germany — [2]Leibniz Institute of Polymer Research Dresden, Hohe Str. 6, 01069 Dresden, Germany — [3]Department of Physics, Mansoura University, Mansoura 35516, Egypt

Forces of interaction within single pairs of poly(2- vinylpyridine) (P2VP) grafted colloids have been measured by optical tweezers (OT) with an extraordinary resolution of *0.5 pN. Parameters to be varied are the concentration and type of salt (KCl, CaCl2, and LaCl3) of the surrounding medium as well as its pH. The observed force-distance relation is quantitatively described by the Jusufi model [Colloid Polym. Sci. 2004, 282, 910-917] for spherical polyelectrolyte brushes which takes into account the entropic effect of the counterions and enables one to estimate the ionic concentration inside the brush. The transition from an osmotic to the salted brush regime is analysed in detail. For the scaling of the brush height a power law is found having an exponent of 0.24*0.01 which ranges between the values expected for spherical and planar brushes. At pH 4 a strong transition from a brush to a pancake conformation takes place.

CPP 37.11 Wed 17:30 Poster B2

Interactions in Thin Aqueous Film of Colloidal Suspensions — ●Yan Zeng and Regine von Klitzing — Stranski-Laboratorium, Department of Chemistry, TU Berlin, Strasse des 17.Juni 124, D-10623 Berlin

Colloidal suspensions are omnipresent in daily life and have many technical applications. To understand the interactions between particles in thin film of colloidal suspensions, we perform force measurements by using Colloidal Probe Atomic Force Microscopy (CP-AFM), in which particles show oscillatory force due to the layer formations of particles under spatial confinement. The distance of layers can be figured out from the force profiles and compared with the mean particle distance obtained from Small Angle X-Ray Scattering (SAXS). Thus we know the structuring of colloidal suspensions can be survived from 3D to 2D or not? Particle concentration, particle size and ionic strength of suspensions have been studied both by CP-AFM and SAXS. The effects of Surface charge and surface elasticity have been studied as well by replacing the solid silicon wafer with mica sheet, air/liquid interface, and modified silicon with polyelectrolyte adsorbed layers. Those are measured by CP-AFM and compared with results from Thin Film Pressure Balance (TFPB) in which particle suspensions form thin films between fluid interfaces and shows no dependency of step size on the particle concentrations. The effect of charge on nanoparticles is studied by adding non-ionic surfactants into particle suspensions and by using non-ionic surfactant itself at concentrations above CMC. Latter case shows significant different result as that of charged particles.

CPP 37.12 Wed 17:30 Poster B2

Photothermal Correlation Spectroscopy and Hot Brownian Motion — ●Romy Radünz[1], Daniel Rings[2], Klaus Kroy[2], and Frank Cichos[1] — [1]Molecular Nanophotonics Group, University of Leipzig — [2]Soft Matter Theory Group, University of Leipzig

Photothermal correlation spectroscopy (PhoCS) is a recently developed tool to explore the diffusion of non-fluorescent tracers of only a few nanometers in size in solution in an equivalent way as it is done in fluorescence correlation spectroscopy. As a key feature of photothermal detection techniques the tracers and their intermediate surrounding are heated up. Although small temperature rises at the particles surface of a few Kelvin are sufficient to detect a single particle, in the case of gold nanoparticles surface temperature rises up to a few 100 K can be achieved with moderate heating intensities exploiting the high absorption cross sections near the plasmon resonance. To interpret the results of PhoCS correctly it is crucial to describe the diffusion of hot particles in a cold surrounding accurately. A model is presented for this Hot Brownian Motion that handles not only the influence of the inhomogeneous viscosity around the particle on the drag coefficient but gives also a first approach to quantify the impact of the non-uniform temperature distribution on the strength of thermal fluctuations that drives Brownian motion. To validate the theoretical description we have studied the diffusion of gold nanoparticles in water. Comparison with the theoretical estimates shows good agreement for temperature rises below 100 K leading to a robust basis for photothermal tracer techniques.

CPP 37.13 Wed 17:30 Poster B2

Temperature mapping of gold nanostructures — •Marco Braun, Romy Radünz, and Frank Cichos — Molecular Nanophotonics Group, University of Leipzig, Linnéstraße 5, D - 04103 Leipzig

Local temperature control on the micro and nanoscale is of interest in many areas in nanotechnology. Heat generated in gold nanostructures when illuminated at their plasmon frequency is transferred into the surrounding medium, what causes a local temperature field and thus a change of physical properties. This is used e.g. in photothermal microscopy to image metal nano particles with the size of a few nano meter. For an application in engineering or biology this temperature fields must be quantified. As a first approach we present a method for rapid temperature mapping using steady-state fluorescence polarization anisotropy (FPA) of dye molecules in a viscous medium covering the plasmonic structures. Polarization anisotropy scales with rotation correlation time and hence with temperature. FPA is measured in a widefield microscope where the polarizations of the fluorescence light are separated. We demonstrate the temperature mapping with gold nano particles immobilized on a glass substrate forming different structures.

CPP 37.14 Wed 17:30 Poster B2

Impact of droplets on thin free standing smectic films — •Sebastian Baumgarten, Thomas John, Kirsten Harth, and Ralf Stannarius — Institut für Experimentelle Physik, Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

Free standing smectic films are stable quasi two-dimensional fluid objects. They have submicrometer thicknesses and consist of layers of smectic liquid crystals. The surface of the films is uniform on the order of single smectic layers.

Picoliter water/glycerol droplets are generated on demand with a piezoelectric dispenser. Their diameters are approximately 30 μm. The position controlled impact of the droplets on the films is observed with a microscope in reflection. Dependent on the materials used, we observe an integration of the droplets in the film structure or a rapid rupture of the free standing film. We record impact and subsequent motion of the droplets in the film with a high speed camera. On an oblique film, the motion of the droplets is gravity driven. This allows a study of hydrodynamics in quasi two dimensions and the viscous drag on the droplet. We plan to have results from variable gravity experiments from DLR parabolic flights at the time of the meeting.

CPP 37.15 Wed 17:30 Poster B2

Single Colloid Electrophoresis in the Presence of Multivalent Counterions — •Shervin Raafatnia and Christian Holm — Institute for Computational Physics, Stuttgart University, Pfaffendwaldring 27, 70569 Stuttgart, Germany

We study the electrophoretic behaviour of a single colloidal particle by simulation. We take into account hydrodynamic interactions via a Lattice Boltzmann fluid. A raspberry-like model is used for the colloidal particle in order to couple it to the fluid.

The electrophoretic behaviour depends on the concentration and valency of counterions in the suspension. Charge inversion, that will lead to a mobility reversal, is expected for multivalent counter ions, because many oppositely charged counterions attach to the colloid.

CPP 37.16 Wed 17:30 Poster B2

Event-driven simulation of spherical colloids with ultra short-ranged attractive interactions in a slit-pore geometry — •Helge Neitsch and Sabine Klapp — Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

We have performed event-driven molecular dynamic investigations of a system consisting of colloidal particles with ultra short-ranged attractive interactions which are confined by two smooth, parallel walls. The pairwise interaction between the particles is modeled using a square-well potential with an attraction length of 4% of the particle diameter. We investigate structural and dynamical properties via quantities like cluster-mass distributions and mean square displacements for the bulk and the confined system using wall distances down to 3 particle diameters. We also present first data for a confined valence-limited model, where particles are allowed to form reversible bonds with a fixed maximum number of neighbors as described in detail in [1].

[1] E. Zaccarelli, J. Phys.: Condens. Matter 19, 323101 (2007)

CPP 38: Micro and Nanofluidics II

Time: Thursday 9:30–10:45 Location: H39

CPP 38.1 Thu 9:30 H39

Droplet and cell sorting in microfluidic channels by surface acoustic waves — Thomas Franke[1,2], Lothar Schmid[1], Susanne Braunmüller[1], Achim Wixforth[1], and •David Weitz[2] — [1]Universität Augsburg, EP1, Microfluidics Group, Augsburg — [2]Harvard University, SEAS, Cambridge, USA

We direct the motion of droplets in microfluidic channels using a surface acoustic wave device. This method allows individual drops to be directed along separate microchannel paths at high volume flow rates, which is useful for droplet sorting. The same principle can be applied for biological cell sorting which operates in continuous flow at high sorting rates. The device is based on a surface acoustic wave cell-sorting scheme and combines many advantages of fluorescence activated cell sorting (FACS) and fluorescence activated droplet sorting (FADS) in microfluidic channels. It is fully integrated on a PDMS device, and allows fast electronic control of cell diversion. We direct cells by acoustic streaming excited by a surface acoustic wave which deflects the fluid independently of the contrast in material properties of deflected objects and the continuous phase; thus the device underlying principle works without additional enhancement of the sorting by prior labelling of the cells with responsive markers such as magnetic or polarizable beads. Single cells are sorted directly from bulk media at rates as fast as several kHz without prior encapsulation into liquid droplet compartments as in traditional FACS. We have successfully directed HaCaT cells, fibroplasts from mice and MV3 melanoma cells.

CPP 38.2 Thu 9:45 H39

Stability of Nanobubbles — •Ralf Kaminke and Klaus Mecke — Institut für Theoretische Physik I, Staudtstr. 7, D - 91058 Erlangen

Gas nanobubbles on substrates were expected to be unstable due to a large Laplace pressure. But AFM images combined with infrared spectroscopy confirmed that they exist and that they are relatively stable [Zhan et al., Phys. Rev. Lett. 98, 136101 (2007)]. As they are not observable in bulk liquids, the substrate must play an important role and therefore density functional theory is the appropriate approach. The bubbles are modelled by spherical caps of nanometer thickness on a flat substrate, so that pressure and density inside the cap is determined by the substrate potential. The gas density is influenced by the substrate strength, the contact angle and the liquid density outside the cap. For a given radius of the spherical cap it is possible to find a contact angle, which minimizes the grand canonical potential and gives a metastable or stable solution depending on the size of the cap. This explains the existence of nanobubbles by substrate potentials.

CPP 38.3 Thu 10:00 H39

Equilibrium properties of polymer films and droplets — •Nikita Tretyakov and Marcus Müller — Institut für Theoretische Physik, Georg-August-Universität Göttingen

We study equilibrium properties of polymer films and droplets on a substrate by Molecular Dynamics simulation. We use a Lennard-Jones bead spring model for polymer chains and the substrate is represented by 2 layers of an fcc lattice. We use a dissipative particle dynamics (DPD) thermostat in our simulation. Various strengths of polymer-substrate interaction were used in order to tune the wettability.

The pressure tensor was calculated for different thicknesses of polymer films using a slab geometry. The values of the surface tensions of the substrate-liquid and liquid-vapor interfaces were derived. The wetting transition between complete (films) and partial wetting (droplets) was observed and the interface potential as function of thickness of the film was computed. The interface potential provides information about the contact angle and the stability of a thin film with respect to dewetting (spinodal or nucleation mechanisms). For ultra-thin films, no homogeneous layer can be observed and in this region the interface potential is a linear combination of contributions from the coexisting thin and thick films.

CPP 38.4 Thu 10:15 H39

Fluid-surface interaction models in Lattice-Boltzmann simulations — •Calin Dan[1], Martin Hecht[1,2], and Jens Harting[1,3] — [1]Institute for Computational Physics, Universität Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart, Germany — [2]High Performance Computing Center, Universität Stuttgart, Nobelstraße 19, 70569 Stuttgart, Germany — [3]Department of Applied Physics, Technische Universiteit Eindhoven, Den Dolech 2, 5600 MB Eindhoven, The Netherlands

An accurate description of fluid-surface interactions is critical for simulations of microfluidic setups. The Molecular Dynamics method is preferred by many researchers to simulate the related phenomena, but these simulations are computationally extremely demanding. Alternatively, the Lattice-Boltzmann method can model the complex phenomena taking place at fluid-surface interfaces by applying for example a phenomenological model, which is based on the well-known Shan-Chen multi-component Lattice-Boltzmann model. However, it is a priori not clear how the influence of parameters like the temperature, charges, or impurities can be taken into account. In this work, we investigate the formulation of fluid-surface interactions within the Lattice-Boltzmann method and quantitatively compare our results to Molecular Dynamics simulations. We calibrate our model parameters using surface tension measurements and apply different implementations to investigate the behavior of a droplet in a capillary with complex fluid-surface interactions.

CPP 38.5 Thu 10:30 H39

Lattice Boltzmann simulations of a sphere approaching a superhydrophobic surface — •Christian Kunert[1] and Jens Harting[2] — [1]Institut für Computerphysik, Pfaffenwaldring 27, 70569 Stuttgart — [2]Dept. of Applied Physics, TU Eindhoven, Postbus 513, NL-5600MB Eindhove

When an object that is submerged in a liquid is approached towards a surface, the lubrication force raises. The measurement of the lubrication force allows to study the flow profile near objects and thus to deduce the flow boundary condition. In particular, such a measurement can be used to study the effect of boundary slippage. The slip on a surface can be increased by combining roughness and hydrophobic interactions. On such surfaces, vapor or gas might be trapped between the roughness asperities creating a so-called superhydrophobic surface. In this contribution we present lattice Boltzmann simulations of a sphere that approaches a superhydrophobic surface generated by bubbles that are trapped in holes on the surface.

CPP 39: Glasses and Glass Transition II (jointly with DY and DF)

Time: Thursday 9:45–12:30 Location: H38

CPP 39.1 Thu 9:45 H38

Dynamics of soft spheres beyond the hard-sphere limit — •Michael Schmiedeberg and Andrea J. Liu — University of Pennsylvania, Department of Physics and Astronomy, 209 South 33rd Street, Philadelphia, PA 19104-6396, USA

In the limit of low pressures the dynamics of model glass-forming liquids with finite-ranged repulsive interactions are universal. In that limit, where the product of the pressure and the particle volume is small compared to the interaction energy, soft sphere systems behave as hard spheres, so that the dynamics correspond to those of the hard-sphere glass transition and depend only on the ratio of temperature to the product of pressure and the particle volume. However, at higher pressures relative to the interaction energy, there are deviations from this universal behavior that depend on the inter-particle potential. We consider a bidisperse system consisting of soft spheres that repel each other according to a power law potential δ^α where δ is the particle overlap. By using molecular-dynamics simulations, we determine relaxation times as a function of temperature and pressure. We find that the deviations from hard-sphere behavior can be collapsed onto a single curve that depends on $p^{1/\alpha}$.

CPP 39.2 Thu 10:00 H38

Correlation between the Diffusion Dynamics and Vibrational Modes of a Model Glass Former — •Oliver Rubner and Andreas Heuer — Institute of Physical Chemistry, University of Münster, Corrensstr. 30, D-48149 Münster, Germany.

In this work we investigate the vibrational modes from computer simulations on a 65 particle binary Lennard-Jones Mixture (BMLJ65) and compare them with the self diffusion dynamics of the particles. As a measure for the dynamics we use the propensities per particle as obtained from an isoconfigurational ensemble which has been introduced by Harrowell (PRL 93, 135701 (2004))

The diffusion dynamics can also be explained in terms of waiting times of the system in inherent structures or metabasins. We compare these waiting times to the vibrational frequencies of the corresponding inherent structures. From this analysis we present the time dependence of the vibrational frequencies which can give some insight into the underlying potential energy surface on which the motion of the system takes place.

CPP 39.3 Thu 10:15 H38

Assessing the predictive power of the Reverse Monte Carlo Method for amorphous systems — •Christian Robert Müller[1], Michael Schuch[2], and Philipp Maass[2] — [1]Theoretical Physics II, Technische Universität Ilmenau, 98684 Ilmenau, Germany. — [2]Fachbereich Physik, Universität Osnabrück, 49069 Osnabrück, Germany.

The quality of structural models generated by the Reverse Monte Carlo (RMC) method in a typical application to amorphous systems is investigated. To this end diffraction data from a molecular dynamics (MD) simulation of a lithium silicate glass are calculated and used to generate RMC models with different protocols and starting configurations. This allows us to directly compare structural properties of the RMC models with the original MD structures and hence assess the predictive power of the RMC method. It is found that partial distribution functions and properties on small length scales are well reproduced by the RMC modeling. However, properties in the medium-range order, as, for example, ring size distributions are not well captured. We further show that certain medium-range order features of the RMC models can be a mere consequence of the chosen starting configuration when using commonly applied RMC protocols. Due care therefore has to be exercised when extracting structural features from RMC models in the medium-range order regime and when using corresponding information as a basis for subsequent studies of ion transport properties.

CPP 39.4 Thu 10:30 H38

Dielectric noise pattern of the Debye- and α-process in a monohydroxy alcohol — •Tobias Gamp, Andreas Reiser, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg

Based on the validity of the fluctuation dissipation theorem, dielectric polarization noise spectroscopy allows to measure the dielectric function of a sample electrically non-driven. 2-Ethyl-1-hexanol is one of the prototypical and widely studied glass-forming liquids showing a Debye-like relaxation and the α-peak, the latter associated with the structural relaxation. Since the Debye process is practically invisible in caloric measurements but prominent in conventional dielectric spectroscopy the question whether it could be caused by the presence of electric fields is debated. We show dielectric noise spectra - both voltage and current power spectral densities - and conventional dielectric spectra. Within our experimental resolution and the validity of the fluctuation dissipation theorem both sets of data are in agreement, indicating that the presence of an external field is not necessary for the occurrence of such a Debye peak.

CPP 39.5 Thu 10:45 H38

Glass transition in high dimensions — •Bernhard Schmid and Rolf Schilling — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany

We have studied the glass transition of hard spheres with diameter σ for dimensions $d \to \infty$ in the framework of mode-coupling theory (MCT). Assuming that the direct correlation function equals the Mayer function in the limit of high dimensions, we have solved numerically the MCT equations [1] up to $d = 800$. The numerical results for the critical collective and self nonergodicity parameters $f_c\,(k;d)$ and $f_c^{(s)}\,(k;d)$ exhibit no Gaussian k-dependence even for $d = 800$. Instead they can be represented by a master function, which vanishes for $k\sigma > \hat{k}_0 d^{3/2}$ with $\hat{k}_0 \cong 0.15$. Inspired by these results, we were able to prove analytically that $f_c\,(k;d)$ converges to $f_c^{(s)}\,(k;d)$ for $k\sigma = O\,(d)$ and $d \to \infty$ and that the critical packing fraction is given by $\varphi_c\,(d) \sim d^2 2^{-d}$. The non-Gaussian character of $f_c\,(k;d)$ and $f_c^{(s)}\,(k;d)$ implies that the hard sphere glass at $\varphi_c\,(d)$ is not a harmonic solid, even in the limit of high dimensions.

[1] M. Bayer, J.M. Brader, F. Ebert, M. Fuchs, E. Lange, G. Maret, R. Schilling, M. Sperl and J.P. Wittmer, Phys. Rev. E **76**, 011508 (2007)

CPP 39.6 Thu 11:00 H38

Brownian dynamics simulation of extensional shear flow in dense colloidal hard-sphere systems — •Olaf Herbst[1] and Thomas Voigtmann[1,2] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — [2]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

Using a novel algorithm based on on event-driven MD simulations adapted for Brownian dynamics, we examine an extensional flow of colloidal particles with periodic boundary conditions. We study the slow dynamics of dense hard-sphere systems when shear rates are high enough to interfere with the slow (alpha) relaxation time. Characteristic features such as the mean-square displacement as a function of time will be discussed for a variety of system parameters.

CPP 39.7 Thu 11:15 H38

The influence of the method of glass preparation and ambient conditions on diffusion of alkaline-earth ions in mixed cation glasses — •Michael Grofmeier and Hartmut Bracht — Institut für Materialphysik, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Str. 10, 48149 Münster

Diffusion of alkaline-earth ions in mixed alkali (A) alkaline-earth (M) glasses of the composition xA2O*(3-x)MO*4SiO2 with 0<x<3 was investigated by means of the radiotracer diffusion technique below the respective glass transition temperatures. Our previous studies reveal a distinct dependence of the diffusion behavior of the alkaline-earth ions on the composition x and type of cations in the glass. Additional experiments on the alkaline-earth ions mobility in sol-gel derived glasses of the same composition were performed in this work in order to determine whether the mixed cation effect in alkali-alkaline-earth silicate glasses also holds for sol-gel derived thin glass films. We found that the diffusion behavior of cations in mixed cation silicate glasses is independent of the way of glass preparation. Further diffusion measurements under reducing atmosphere demonstrate a retarded mobility of the alkaline-earth cations.

CPP 39.8 Thu 11:30 H38

Crystallization and structural investigation of Eu-doped fluorozirconate-based glass ceramics. — •Christian Passlick[1], Bernd Ahrens[1,2], Bastian Henke[1,2], Jacqueline A. Johnson[3], and Stefan Schweizer[1,2] — [1]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale) — [2]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale) — [3]Department of Materials Science and Engineering, University of Tennessee Space Institute, Tullahoma, TN 37388, USA

A series of Eu-doped fluorozirconate-based glass ceramics has been developed for medical and photovoltaic applications. In the first case, the materials can be used as x-ray scintillators or x-ray storage phosphors, in the latter case as down-converting top layers for highly efficient solar cells. The glasses are based on a modified ZBLAN composition, i.e. a mixture of Zr, Ba, La, Al, and Na fluorides. They are additionally doped with chlorine ions to initiate the growth of $BaCl_2$ nanocrystals upon thermal processing. Eu^{2+} ions are incorporated into the nanocrystals during the annealing procedure enabling a strong fluorescence upon ultraviolet or x-ray excitation. The nanocrystal size and structural phase depend significantly on the heating conditions and Eu doping level. X-ray diffraction patterns show a structural phase change of the $BaCl_2$ nanocrystals from hexagonal to orthorhombic as annealing temperatures are increased. DSC experiments were performed to obtain activation energies, thermal stability parameters and information on the crystal growth mechanisms.

CPP 39.9 Thu 11:45 H38

Time-resolved optical spectroscopy on Er-doped fluorozirconate-based glasses for efficient up-conversion — •Ulrich Skrzypczak[1], Manuela Miclea[1], Jacqueline A. Johnson[2], and Stefan Schweizer[1,3] — [1]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale) — [2]Department of Materials Science and Engineering, University of Tennessee Space Institute, Tullahoma, TN 37388, USA — [3]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale)

Fluorozirconate(FZ)-based glasses have shown their potential as hosts for rare-earth (RE) ions such as Er, in these glasses REs show emissions that would be quenched in other glasses. Such material systems are of practical interest for photon up-conversion. For photovoltaic applications, the efficiency of bifacial solar cells could be vastly improved by an up-converting back layer. Up-conversion is the sequential absorption of two or more low-energy infrared photons by a RE ion followed by subsequent emission of a visible photon. This process is dependent on the intermediate level lifetime of the RE ion, which is determined by the phonon energies of the host material. Low phonon energy glasses like FZ glasses are thus desirable hosts. The lifetimes of the energy levels involved in the up-conversion process are investigated by time-resolved spectroscopy. Short laser pulses at different wavelengths are used for excitation; the emissions are detected via time-correlated photon counting. The radiative and non-radiative decay processes in Er-doped FZ glasses are analyzed and discussed.

CPP 39.10 Thu 12:00 H38

Spectral down-conversion in Sm-doped borate glasses for photovoltaic applications — •Marcel Dyrba[1], Paul-Tiberiu Miclea[2,3], and Stefan Schweizer[1,2] — [1]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale) — [2]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale) — [3]Institute of Physics, Martin Luther University of Halle-Wittenberg, Heinrich-Damerow-Str. 4, 06120 Halle (Saale)

Samarium fluorescence in glasses has attracted much attention in the past two decades, in particular for studies on spectral-hole burning, excited state absorption, and laser properties. Here, a class of Sm-doped borate glasses has been developed for photovoltaic applications. The fluorescent glass is placed on top of a solar cell and, in the case of Sm^{3+} doping, converts the incident violet/blue part of the solar spectrum to red light which is more efficiently absorbed by the solar cell. The chemical base composition of borate glasses consists of the network former boron oxide and metal oxides as network modifiers. The spectroscopic properties of Sm^{3+}, in particular the fluorescence efficiency, are significantly influenced by the electron negativity of the network modifier. Some of the glasses are additionally doped with silver oxide. Subsequent heat treatment causes reduction of the doped silver ions and leads to the formation of metallic silver nanoparticles. The effect of the local field enhancement around the Sm^{3+} ions, which is due to surface plasmons from the silver nanoparticles being close by, is investigated.

CPP 39.11 Thu 12:15 H38

Raman spectroscopy on barium halide nanoparticles in fluorozirconate-based glasses — •Charlotte Pfau[1], Paul-Tiberiu Miclea[2,3], and Stefan Schweizer[1,2] — [1]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale) — [2]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale) — [3]Institute of Physics, Martin Luther University of Halle-Wittenberg, Heinrich-Damerow-Str. 4, 06120 Halle (Saale)

Rare-earth(RE) doped fluorozirconate-based glasses show enhanced fluorescence properties when they are additionally doped with Cl or Br ions, which initiate the growth of $BaCl_2$ or $BaBr_2$ nanocrystals, respectively, upon thermal processing. The REs are incorporated into the nanocrystals during the annealing procedure enabling a strong fluorescence upon excitation. A critical parameter for the fluorescence efficiency is the non-radiative decay process from the excited to the ground state. Non-radiative decay processes are determined by the phonon energies of the host system. Low phonon energy systems such as $BaCl_2$ or $BaBr_2$ are desirable hosts for fluorescent ions. The size and structural phase of the nanocrystals depend significantly on the heating conditions; consequently, a series of chlorine- or bromine-doped fluorozirconate-based glasses were analyzed to determine their phonon energy spectra by Raman spectroscopy. For comparison, the phonon spectra of bulk $BaCl_2$, and $BaBr_2$ were investigated.

CPP 40: Nanoparticles and Composite Materials I

Time: Thursday 9:30–12:45 Location: H48

CPP 40.1 Thu 9:30 H48

Investigation of Structure and Miscibility Patterns of Gold-Platinum Nanoparticles — •Linn Leppert and Stephan Kümmel — Institute of Theoretical Physics, University of Bayreuth, Germany

Gold-platinum nanoparticles (NPs) immobilised within spherical polyelectrolyte brushes have been proven to be excellent catalysts of oxidation reactions, being more efficient than pure NPs from gold or platinum [1]. However, little is known about their geometrical and electronical structure, as well as about the way the catalytic mechanism works. The theoretical treatment of these systems is complicated by the large number of electrons and the necessity to account for relativistic effects.

We present structure and miscibility patterns of small gold-platinum NPs obtained from numerical calculations. Our technique combines density functional theory based Simulated Annealing and local optimization methods and offers numerical efficiency as well as the inclusion of scalar relativistic effects.

[1] M. Schrinner et al., Advanced Materials 2008, 20, 1928-1933.

CPP 40.2 Thu 9:45 H48

Fibre-like polymer-metal nanocomposites - the morphology of a gold layer on curved polymer surfaces — •Stephan V. Roth[1], Rainer Gehrke[1], Ulla Vainio[1], Kai Schlage[1], Ralf Röhlsberger[1], Manfred Burghammer[2], Christian Riekel[2], Volker Körstgens[3], Ezzeldin Metwalli[3], and Peter Müller-Buschbaum[3] — [1]HASLYAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany — [2]ESRF, 6rue Jules Horowitz, F-38043 Grenoble, France — [3]Physik-Department E13, TU München, James-Franck-Str. 1, D-85748 Garching, Germany

Polymer-metal nanocomposites are used in many areas of sensor techniques, information technology and biotechnology [1].These devices exploit the plasmon resonances of the confined electron gas in the metal nanostructures and typically exhibit a flat geometry. However, using aligned cylindrical, wire- or stripe-like arrays of nanoparticles enables to install plasmon waveguide devices which allow for guiding electromagnetic energy below the diffraction limit of light [2]. In our approach we use a two step technique to produce a scalable stripe-like flexible geometry. We indent a scalable biofibre in a polymer film - creating a polymeric channel - and subsequently deposit metal via sputter-deposition [3]. We follow the topography of the metal layer through the cross-section of the polymeric channel. Our findings show a strong correlation of nanoparticle morphology and cross-sectional position.

[1] Wolkenhauer et al., Appl. Phys. Lett. 89 (2006) 054101 [2] Maier et al., Nature Mat. 2, 229 (2003) [3] Metwalli et al., Langmuir 24, 4265 (2008)

CPP 40.3 Thu 10:00 H48

Directed Self-Assembly of Nanoporous Metallic- and Bimetallic Nanoparticle Thin Films — •Torsten Pietsch[1], Nabil Gindy[2], and Amir Fahmi[2] — [1]Fachbereich Physik, Universität Konstanz, Universitätstraße 10, 78464 Konstanz, Germany — [2]Department of Mechanical, Materials and Manufacturing Engineering, University of Nottingham, University Park, Nottingham, NG7 2RD, United Kingdom

Nanoporous thin films attracted considerable interest due to potential applications in optical coatings, catalysis, sensors as well as electronic devices. Recently, such films were prepared by post deposition treatments. The present study is focused on the fabrication of nanoporous thin films via directed self-assembly of hybrid materials.[1] Due to the nature of this process no additional treatments are necessary to develop the pores.[2] Hierarchical nanoporous structures are fabricated directly via deposition of polymer templated Au-nanoparticles onto hydrophilic substrates.[3] These films exhibit two different pore diameters and a total pore density of more than 10^{10} holes per cm^2. Control over the pore size is achieved by changing the molecular weight of the PS-b-P4VP diblock copolymer. Moreover, the porous morphology is used as a template to fabricate bimetallic nanostructured thin films. Such well-defined nanostructures, not only exhibit unique physical properties but also provide control over the hydrophobicity of the coated surfaces.

[1] Pietsch T et al., Macromol. Chem. and Phys. 210 (2009) 864

[2] Pietsch T et al.; Soft Matter 5 (2009) 2188

[3] Fahmi A et al.; Macromol. Rap. Comm. 38 (2007) 2300

CPP 40.4 Thu 10:15 H48

Real time GISAXS study of magnetic nanoparticle assemblies on polymer templates — •Ezzeldin Metwalli[1], Kai Schlage[2], Volker Körstgens[1], Sebastien Couet[2], Robert Meier[1], Gunar Kaune[1], Stephan V. Roth[2], Ralf Röhlsberger[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physikdepartment E13, 85747 Garching — [2]HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany

Hybrid materials consisting of metal nanoparticles dispersed in a polymer matrix[1,2] open pathways for engineering composites that exhibit advantageous electrical, optical, and magnetic properties. Using a portable DC magnetron sputtering deposition system, the incorporation of cobalt atoms into a microphase-separated polystyrene-block-polyethylene oxide P(S-b-EO) diblock copolymer film with parallel cylinder morphology is achieved. Time-resolved in situ grazing incidence small angle X-ray scattering (GISAXS) allows successfully to systematically investigate the formation and growth of Co nanoparticles into the polymer template. Cobalt atoms were found to wet selectively the polystyrene domains of the microphase-separated polymer film and then aggregate to form surface metal nanopatterns. Upon increasing the amount of metal content, the selectivity nature of the sputtering process was found to diminish with the formation of a pseudo-uniform metal layer. [1] E. Metwalli et al., Langmuir 24, 4265 (2008) [2] E. Metwalli et al., Langmuir 25, 11815 (2009)

CPP 40.5 Thu 10:30 H48

Manufacturing of barium titanate thin films with designed microstructure by a sol-gel process: in-situ SAXS investigation of the precursor system — •Tomasz Stawski, Sjoerd Veldhuis, Johan ten Elshof, Ole Göbel, Hessel Castricum, and Dave Blank — University of Twente, Inorganic Materials Science group, P.O. Box 217, 7500 AE Enschede, The Netherlands

Barium titanate (BTO) is used as a high-k dielectric material in multilayer ceramic capacitors. The minimum BTO layer thickness that can be achieved commercially with the state of the art tape casting methods is about 1 um, which implies the use of starting powders with a particle size of ca. 200 nm. Further downsizing requires finer powders. Wet-chemical methods based on sol-gel reactions are among most thoroughly investigated, and can also be applied to make BTO. Knowledge of the size, shape and kinetics of primary sol-gel derived oligomeric nanostructures in solution is crucial to optimize the processing of functional oxide thin films from these solutions. The barium titanate sol-gel precursor system was analyzed by small angle X-ray scattering analysis at the DUBBLE beamline at the ESRF in Grenoble. BTO sols were formed in the reaction of barium acetate, tit! anium isopropoxide and water in glacial acetic acid and 2-methoxyethanol. The relationship between size and dimensionality of the oligomers, and the influence of synthesis conditions (temperature, concentrations of reactants) were investigated. Evolutionary, systematic changes in the radii of gyration (Rg) and internal structure of colloidal sols (characterized by the fractal dimension, Df) were monitored as a function of time.

15 min. break

CPP 40.6 Thu 11:00 H48

Dynamics of entangled Polyisoprene-POSS Nanocomposites studied by Dielectric Spectroscopy and Linear Rheology — •Thomas Glomann[1,2], Klaus Nusser[1,2], Gerald Johannes Schneider[2], Wim Pyckhout-Hintzen[1], Reiner Zorn[1], Lutz Willner[1], Juergen Allgaier[1], and Dieter Richter[1] — [1]IFF, Forschungszentrum Jülich GmbH, 52425 Jülich — [2]Jülich Centre for Neutron Science at FRM2, 85747 Garching

Filler particles can tremendously improve the macroscopic properties of polymeric substances attributing to the enormous technological importance of composite materials. Recently, it was found that the addition of nanosized particles can lead to new and unexpected effects like a huge drop in viscosity. The microscopic details of the complex polymer-filler interactions still lack a general understanding.

We investigated the dynamics of entangled polyisoprene in the presence of POSS (polyhedral oligomeric silsesquioxanes) nanoparticles at different filler loadings by means of dielectric spectroscopy and linear rheology. The dielectric measurements reveal that the particles do not alter the observed microscopic chain dynamics at all. However, the mechanical properties show a strong increase in modulus strength with increasing filler concentration. Moreover, the liquid-like behavior at low frequencies changes to a solid-like behavior above a certain critical filler level.

CPP 40.7 Thu 11:15 H48

Influence of the nanoparticles on the structural relaxations in epoxy nanocomposites as seen by rheological spectroscopy — •Matthieu Thomassey, Jörg Baller, 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

Due to their large surfaces nanoparticles are well known to have a dramatic influence on the glass transition behavior of nanocomposites made of oligomer matrices and inorganic fillers. Generally one distinguishes between topological and surface induced effects of the nanoparticles. By changing the concentration of the filler particles, topological constraints are expected to have an influence on the glass transition of the composite. By modifying the state of their surfaces the interaction between the oligomer molecules and the nanoparticles and hence the mechanisms leading to the glass transition are also altered. This paper presents a rheological study of an epoxy resin (DGEBA) filled either with alumina particles with a hydrophilic surface or silica with a hydrophobic surface. Topological and surface-induced effects of the nanoparticles on the glass transition behavior of the composite are elucidated. Rheological spectroscopy is used to study the temperature and frequency dependencies of the shear moduli for the two types of nanocomposites. Special attention is paid to an abnormal behavior of the real and imaginary parts of the shear modulus.

CPP 40.8 Thu 11:30 H48

Polymer-grafted Silica Nanoparticles: a Structural Characterization in Solution and Bulk — •Mathias Meyer[1], Eike Hübner[1], Wim Pyckhout-Hintzen[1], Jürgen Allgaier[1], Aurel Radulescu[2], Dieter Richter[1,2], Pieter J. in 't Veld[3], and Horst Weiss[3] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich GmbH — [2]Jülich Centre for Neutron Science, Garching, Forschungszentrum Jülich GmbH — [3]BASF SE, Ludwigshafen

Though nanocomposites with their astonishing properties are of great interest for research and industry, microscopic details of the polymer-interface have been scarcely investigated. Therefore a model system basing on grafted silica nanoparticles is designed and studied. From TEM, SANS and SAXS experiments, particle sizes and their distribution were determined independently. Despite surface stabilization, attractive inter-particle interactions, formerly neglected in literature, lead to small dynamic aggregates, which we described microscopically in a consistent manner. The influence of the grafting density and the chain length and type of the graft as well as of the dispersing medium were investigated in terms of a polydisperse core-shell-type model. Our experimental results are compared to multiscale simulations within an EU FP7 project (NanoModel), focussing on the radial density profile of the polymer shell. Due to our newly developed "grafting to" approach a labelling of the grafted chains is now possible, which allows for the first time to investigate the chain conformation in the shell. Unlike with other grafting methods (i.e. ATRP), also polymers with a low entanglement molecular weight can be grafted to.

CPP 40.9 Thu 11:45 H48

Functionalization and Characterization of SWCNTs for Electronics Applications — Engin Karabudak[1,2], Claudia Backes[3], Frank Hauke[3], Andreas Hirsch[3], and •Wendel Wohlleben[1] — [1]BASF SE, Polymer Physics Research, 67056 Ludwigshafen, D — [2]Present address: MESA+ Research Institute, University of Twente, NL — [3]Department of Chemistry and Pharmacy & ZMP, Universität Erlangen-Nürnberg, 91054 Erlangen, D

We report the application of a novel multiwavelength analytical ultracentrifuge (AUC) to the correlation between hydrodynamic size and absorption in CNT dispersions. The statistical relevance is high due to the evaluation of 10^{11} colloids in one experiment. The machine operates at up to 60 krpm and records c(r,t,lambda) with a 100-fold speed improvement over commercial AUCs. Single-wall CNTs are notoriously difficult to disperse, not only because of their high tendency to agglomerate, but also due to insufficient understanding of the CNT-ligand interactions. Here we prepare an up to 88 percent efficient dispersion of SWCNTs (HiPco and CoMoCAT) by non-covalent ligands (perylene bisimides with Newkome dendrimers) and intercalant agents (perylenes). Without previous purification we quantify from a single 1h-experiment the coexistence of debundled, ligand-encapsulated CNTs; CNT bundles with few ligands attached; hydrolyzed intercalant; intercalant - ligand micelles, with the absorption profiles and anhydrous specific volume for each component. Bulky dendritic groups on the surfactants systematically reduce the adsorption density on the CNT surface, which is on the order of 1 mmol surfactant / g SWCNT.

CPP 40.10 Thu 12:00 H48

Modelling of electric conductivity in sheared CNT/polymer composites — •Marina Saphiannikova[1], Tetyana Skipa[2], Dirk Lellinger[2], Ingo Alig[2], and Gert Heinrich[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden — [2]Deutsches Kunststoff Institut, Schlossgartenstr. 6, 64289 Darmstadt

Theoretical description of electric properties of the polymer melts, filled with attractively interacting conductive particles, represents a great challenge. Such filler particles tend to build a network-like structure [1] which is very fragile and can be easily broken under steady shear flow with shear rates of about 1/s. In the quiescent state of melt the particles agglomerate again, slowly restoring the network structure. The agglomeration process can be facilitated by application of shear flow with small shear rates of about 0.01/s [1]. In this study, the shear-induced changes in electric conductivity of polymer composites are described using a Bethe-lattice percolation theory [2] which enables the modelling of filler network conductivity. Additionally, we take into account the matrix conductivity enhanced by the presence of single filler particles. The percolation theory is coupled with a kinetic equation for the scalar structural parameter which describes the instantaneous state of filler network at particular flow conditions. The coupling approach is verified in transient shear experiments carried out on polycarbonate composites filled with multi-wall carbon nanotubes.

This work was supported by the BMBF grant No.03X0504E.

[1] T. Skipa et al. Phys. Stat. Sol. B 246, 2453 (2009)

[2] F. Semeriyanov et al. J. Phys. A: Math. Theor. 42, 465001 (2009)

Invited Talk CPP 40.11 Thu 12:15 H48

Novel Nanocomposites in Industrial Applications - Chances and Challenges — •Péter Krüger — Bayer MaterialScience AG, Chempark Geb. Q23, 51368 Leverkusen

Zur Zeit nicht verfügbar

CPP 41: Nanoparticles and Composite Materials II

Time: Thursday 14:00–17:15 Location: H48

CPP 41.1 Thu 14:00 H48

Study of the Defect Structure of SnO_2:F Nanoparticles by High-resolution Solid-State NMR — •Yamini Avadhut[1], Johannes Weber[1], Elin Hammarberg[2], Claus Feldmann[2], Inga Schellenberg[3], Rainer Pöttgen[3], and Jörn Schmedt auf der Günne[1] — [1]Department of Chemistry, Munich University (LMU), Munich, Germany — [2]University of Karlsruhe (TH), Germany — [3]Universität Münster, Germany

The defect structure of fluorine doped tin oxide (FTO) nano particles was investigated by using ^{119}Sn,^{19}F and ^{1}H solid-state NMR [1]. FTO is a substitute of indium tin oxide, the most commonly used TCO. Fluorine doping is supposed to increase conductivity and is studied by solid state MAS NMR and ^{119}Sn Mößbauer spectroscopy. Quantitative NMR [2], CPMAS, homonuclear dipolar recoupling and rotational echo double resonance experiments allowed us to study the doping homogeneity, dynamics. On the basis of the experimental results we discussed different models which explain the increase in conductivity of SnO_2:F caused by fluorine doping and refine our view by ab initio calculations of different defect models.

[1] Y.S.Avadhut, J.Weber, E. Hammarberg, C.Feldmann, I.Schellenberg, R.Pöttgen, J.Schmedt auf der Günne in preparation. [2] Y.S.Avadhut, D.Schneider, and J.Schmedt auf der Günne, J. Magn. Reson., 201:1-6, 2009.

CPP 41.2 Thu 14:15 H48

Excitation Dynamics in Polymer-Coated Semiconductor Quantum Dots with Integrated Dye Molecules: The Role of Reabsorption and Radiationless Transfer — •Tobias Niebling, Sebastian Friede, Feng Zhang, Zulquarnain Ali, Wolfram Heimbrodt, and Wolfgang J. Parak — Department of Physics and Material Sciences Center (WZMW), Philipps University Marburg, Renthof 5, D-35032 Marburg, Germany

Colloidal quantum dots can provide a basis for applications in biolabelling and bioanalytics. Inorganic CdSe/ZnS core-shell quantum dots (QDs) were coated with amphiphilic polymers in order to transfer them to aqueous solutions. The polymer shell allows a functionalization of the nanoparticles. In this work ATTO-dye molecules were linked to the QDs. The excitation dynamics within this system have been investigated by steady state and time-resolved optical spectroscopy. (I) Reabsorption of QD emission by the dye molecules and (II) Förster resonant energy transfer (FRET) from the donor QD to the accepting dye molecules dominate the photoluminescence properties. The spectral overlap between the QD emission and the dye absorption and thereby the transfer efficiency can be tuned by the size of the QDs. Our description of the emission behaviour yields a kinetic model that considers the dynamics of the excited QD and dye molecules with respect to the different transfer mechanisms and reveals the respective contributions of reabsorption and radiationless transfer.

CPP 41.3 Thu 14:30 H48

New Insights to Photo-destructive Effects on Quantum Dots — •Danny Kowerko[1], Jörg Schuster[2], and Christian von Borczyskowski[1] — [1]Center of nanostructured materials and analytics, TU-Chemnitz, 09107 Chemnitz — [2]Fraunhofer-Einrichtung für Elektronische Nanosysteme ENAS, Technologie-Campus 3, 09126 Chemnitz

Energy and charge transfer in assemblies of semiconductor quantum dots (QDs) and organic (dye) molecules offer numerous applications in science and technology. The surface properties of CdSe and CdSe/ZnS colloidal QDs play a crucial role for the photoluminescence (PL) properties and thus the respective transfer efficiencies. In our contribution we demonstrate how PL quenching and enhancement are related to the surface. Therefore the influence of oxidation and surface adsorption by perylene bisimide (PBI) molecules will be elucidated by time-resolved ensemble and single particle spectroscopy. Irreversible and reversible spectral blue shifts are discriminated and related to surface and intrinsic modifications of the QD and conclusions for the efficiency of energy transfer are drawn.

CPP 41.4 Thu 14:45 H48

Controlled embedding of semiconducting nanoparticles in a conducting polymer template — •Matthias A. Ruderer[1], Stefan M. Prams[1], Weinan Wang[1], Qi Zhong[1], Robert Meier[1], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department LS E13, James-Franck-Str. 1, 85747 Garching (Germany) — [2]HASYLAB at DESY, Notkestr. 85, 22603 Hamburg (Germany)

Photovoltaic based on organic compounds such as conjugated polymers attracted increasing interest during the last two decades. Beside of all organic systems, the combination of an inorganic and an organic component, so called hybrid composites, have shown promising properties. In a typical hybrid system an inorganic porous template is filled with an organic photoactive material. Our approach is based on the selective embedding of nanoparticles in a diblock copolymer matrix. [1] We use a rod-coil like copolymer, with a photoactive conjugated and a styrene block, as a template for embedding titania nanoparticles which are directed into the coil like part. The structural length is defined by the copolymer and is in the range of the exciton diffusion length which is crucial in organic systems. The evolving structures are investigated with imaging methods like SEM and grazing incidence small angle X-ray scattering (GISAXS). The influence on the optical and electrical properties are investigated with UV/Vis and conductivity measurements and compared with the structural results. [1] M.M.Abul Kashem, J.Perlich, L.Schulz, S.V.Roth, P.Müller-Buschbaum; Macromolecules 41, 2186-2194 (2008)

CPP 41.5 Thu 15:00 H48

Symmetry and Shape dependent Properties of CdSe Nanostructures — •Farzana Aslam[1] and Christian von Ferber[2,3] — [1]Department of Mathematics, Statistics and Engineering Sciences, Coventry University, UK — [2]Applied Mathematics Research Centre, Coventry University, UK — [3]Physikalisches Institut, Universität Freiburg

We investigate the impact of symmetry, shape and size of CdSe particles on their electrostatic and structural properties and discuss consequences for their role as sensitizers. Other than previous theoretical studies which have focussed on a fixed particle shape and a small set of sizes we systematically investigate a large set of more than a thousand nanocrystals with different shapes, sizes, and aspect ratios. This unusual approach allows us to draw conclusions on significant correlations of the relevant properties of these crystals with symmetry, shape, surface character and size. In particular, we find significant differences between the properties of approximately spherically shaped particles, and particles with well defined surfaces along crystal planes but also between particles of the latter class. A surprisingly strong impact of the specific shape and surface configuration is found for the internal structure well inside the crystal as measured by bond lengths correlated with coordination numbers.

CPP 41.6 Thu 15:15 H48

Net Charge on Colloidal CdSe/ZnS Evidots in Nonpolar Solvents — •Nicole Amecke-Mönnighoff and Frank Cichos — Molecular Nanophotonics Group, University of Leipzig, Linnéstraße 5,04103 Leipzig

An interesting and promising class of materials studied over the last years are semiconductor Quantum Dots (QDs). Many applications seek to make use of their favorable fluorescence characteristics, like tunable emission wavelength, high quantum yield and 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 and the quantum confined Stark effect. Those charges can arise from ejection of electron or hole via tunneling leaving behind the counterpart and changing the matrix charge constellation. So far the model, assuming the net charge of a QD plus close surroundings to be zero. When applying an electric field to a solution of QDs in toluene, we surprisingly find a net positive charge on a great part of QDs, even though being dispersed in a nonpolar solvent. As those charged QDs still fluoresce the charge will most likely be located at the surface. Since this surface charge is very unlikely to be formed in the nonpolar toluene, we suggest that it is the result of the synthesis of the QDs. Such a charge should definitely influence blinking and probably all the characteristics mentioned above. It even might bias electron tunneling and should thus be included in blinking models. Our first goal is to find its origin, amount and precise location, including also that of the counter charge.

15 min. break

CPP 41.7 Thu 15:45 H48

Synthesis of stable bimetallic AuAg and CoPd colloids via diblock copolymer micelle nanoreactors — •Willian G. Menezes[1], Volkmar Zielasek[1], Christian Kübel[2], Karsten Thiel[3], and Marcus Bäumer[1] — [1]Universität Bremen, Institut für Angewandte und Physikalische Chemie — [2]Forschungszentrum Karlsruhe / KIT — [3]Fraunhofer IFAM, Bremen

The preparation of metal nanoparticles (NPs) by using block copolymers (BCP) as encapsulating agent yields NPs with narrow size distributions and outstanding control over the inter-particle distance. Various metal salts, also in combination, can be easily loaded as precursor for NPs into the micelle cores.[1] We will demonstrate the synthesis of AuAg and CoPd bimetallic NPs by using PS-*b*-P4VP as stabilizing agent and $N_2H_4{\cdot}H_2O$ as reducing agent. TEM images show spherical crystalline NPs with diameters varying between 3 and 6 nm, for both, AuAg and CoPd. In UV-vis only one plasmon band at 460 nm was observed for Au-Ag NPs, indicating the formation of truly bimetallic NPs. STEM and EDX confirm that single NPs contain both metals, in the case of AuAg with atomic ratios of Au:Ag as 1:1, in agreement with the metal salt concentrations used. In catalysis, bimetallic systems can demonstrate unique properties distinct not only from the bulk metals but also from the corresponding monometallic NPs. The results of first catalytic tests for CO oxidation at titania loaded with AuAg and CoPd NPs prepared via the BCP route will be presented. Despite the organic matrix, the NPs are active for CO oxidation under certain conditions.

[1] S. Förster, M. Antonietti, Adv. Mater. 10 (1998) 195.

CPP 41.8 Thu 16:00 H48

Hybrid raspberry particles for superhydrophobic surfaces — •Doris Vollmer, Maria d'Acunzi, Lena Mammen, and Hans-Jürgen Butt — Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz (Germany)

On superhydrophobic surfaces, water droplets roll off even at inclinations of just a few degrees, taking up any contaminants encountered on their way. In nature, the lotus leaf is one of the most efficient examples of a superhydrophobic surface. Its superhydrophobicity is conferred by surface roughness on the nano- and micrometer scale.

Here we report a novel method to prepare superhydrophobic films from raspberry particles. The term *raspberry particle* refers to the topography of their surfaces with nano-sized secondary spheres attached to a considerably larger primary particle. Our particles consist of a polystyrene core and a rough silica shell. The hybrid nature of our particles offers the possibility to design a completely new approach to prepare superhydrophobic surfaces.

Multilayers of particles are formed by evaporation of the aqueous dispersant. By exposure of the hybrid particles to tetrahydrofuran vapour, polystyrene leaks out of the core and forms bridges between the particles, thereby providing mechanical stability. The films are hydrophobized by silanization with a semifluorinate silane. Films show static contact angle for water of about 160° and roll-off angle of 1°.

CPP 41.9 Thu 16:15 H48

Electron beam-induced nanoparticle formation in Au and Pt salt-loaded polystyrene-block-poly(4-vinylpyridine) micelles — •Volkmar Zielasek[1], Christian Kübel[2], Willian G. Menezes[1], Karsten Thiel[3], and Marcus Bäumer[1] — [1]Universität Bremen, Institut für Angewandte und Physikalische Chemie — [2]Forschungszentrum Karlsruhe/KIT — [3]Fraunhofer IFAM, Bremen

Using diblock copolymer micelles as nanoreactors for the generation of metal colloids has proven to be a universal route to regular arrays of uniformly sized nanoparticles (NPs) for a variety of metals [1]. When PS-*b*-P4VP micelles in toluene are loaded with metal salts, the formation of a single NP in each P4VP core can be achieved in a subsequent reduction step induced either chemically, by plasma or by UV or electron irradiation. We will present a detailed TEM study of metal colloid formation during this reduction step in Au and Pt salt-loaded PS-*b*-P4VP micelles at variable temperature in the range 95 - 300 K. Electron irradiation-induced coagulation of metal and initial formation of particulates with subnanometer diameters within the P4VP cores is observed in the entire temperature range for Au as well as for Pt. Particle coarsening and ripening, however, strongly depend on the metal, the electron dose and, in particular, on temperature. Counterintuitively, the dynamics of metal aggregation into a single NP within each micelle core is faster at low temperature whereas at 300 K even high densities of subnanometer particulates remain stable. Stability of the P4VP is probably essential for metal mobility within the core.

[1] S. Förster, M. Antonietti, Adv. Mater. 10 (1998) 195.

CPP 41.10 Thu 16:30 H48

Ground state structures in ferrofluid monolayers: influence of an external magnetic field — •Taisia Prokopieva[1], Victor Danilov[1], Sofia Kantorovich[1,2], and Christian Holm[2] — [1]Ural State University, Ekaterinburg, Russia — [2]ICP, University of Stuttgart, Stuttgart, Germany

More and more attention is given to ferrofluid monolayers recently because they find different applications in various disciplines. Based on our previous results [Prokopieva et al. Phys. Rev. E (2009), V.80, P. 031404], we investigate the microstructure of ferrofluid thin films at low temperatures under applied external magnetic field. Using a combination of analytical methods and Monte Carlo simulations we have studied the ground state structures in two cases: the field aligned perpendicular and parallel to the layer. The crucial influence of the external field is demonstrated. We find different configurations for different magnetic fields. The critical parameters of structural transitions for different fields are proved to depend on the number of particles in the system.

The results of the ground state structures in the presence of the external field will be used to understand the microstructure of ferrofluid monolayers at room temperatures.

CPP 41.11 Thu 16:45 H48

Ferrofluids With Shifted Dipoles — •Rudolf Weeber, Sofia Kantorovich, Joan J. Cerdà, and Christian Holm — Institute for Computational Physics, Pfaffenwaldring 27, 70569 Stuttgart, www.icp.uni-stuttgart.de

In the last decades, ferrofluids and magnetic colloids have become relevant in many applications ranging from engineering to medicine, and therefore have attracted the interest of scientists from many fields. We present simulations and analytical calculations for a model system for magnetic nanoparticles that have a dipole moment shifted out of the center of mass, towards the surface. I.e., the spherical symmetry of the particle is broken. This model is inspired by experiments on colloidal particles with magnetic caps by Erbe et. al. While it does not attempt to reproduce the experiments exactly, similar structures can be observed already for intermediate shifts of the dipole. In our contribution, we discuss ground state properties for small clusters, which help us to understand the building blocks of larger systems. For moderate shifts of the dipole moment, the ground state structure changes from chains and rings with parallel alignment of moments, usually observed in dipolar particles, to pairs and triangles with close to anti-parallel orientation of moments. We also present magnetization properties of larger systems at finite temperature and observe the influence of the shift in particular on the initial slope of the magnetization curve, namely, the initial susceptibility.

CPP 41.12 Thu 17:00 H48

Molecular Dynamics Simulations of Thermal Decomposition of Methane using a Reactive Force Field — •Norbert Lümmen — University of Bergen, Department of Physics and Technology, Allégaten 55, 5007 Bergen, Norway

Incomplete combustion of carbon based materials produces fine carbon rich particles. Controlled manufacturing of very pure carbon nanoparticles (Carbon Black) can be achieved by, for example, thermal decomposition of gaseous precursors like acetylene or methane.

Molecular dynamics simulations of hydrocarbon growth after noncatalyzed thermal decomposition of methane were carried out in order to understand the impact of the thermal decomposition reaction of methane on the formation of large hydrocarbon molecules and their role in formation of carbon nanoparticles [1]. A reactive force field (ReaxFF [2]) was employed to model the interactions of the involved hydrocarbons.

After thermal decomposition of methane the formation of molecular hydrogen, a broad range of hydrocarbons and carbon dimers was observed. The basic reactions are in agreement with existing models of thermal decomposition of methane. An increasing variety of hydrocarbons is observed with increasing temperature. The largest molecules formed within 1 ns of simulation time contain enough carbon atoms to be able to form 5- or 6-membered carbon ring structures.

[1] Lümmen, submitted for publication.

[2] van Duin et al., J. Phys. Chem. A 105, 9396 (2001).

CPP 42: Colloids and Complex Liquids I

Time: Thursday 11:00–12:45 Location: H39

Topical Talk CPP 42.1 Thu 11:00 H39

Local dynamics near the 2D-Glass Transition in Binary Colloidal Mixtures — •Georg Maret, Florian Ebert, Sylvain Mazoyer, and Peter Keim — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

Micron sized colloidal particles in suspension are ideal model systems to study structural and dynamic properties of condensed matter at 'atomic' scales. This is illustrated by video microscopy experiments on binary mixtures of superparamagnetic colloids which are pinned at the flat horizontal air/water interface[1]. Their pair potential is tuned by an external magnetic field which drives the 2D system from the liquid to the glassy state. We observe competing local crystallites[2], particle motion coupled to cage motion and intra-cage hopping[3] as well as dynamic heterogeneities which are correlated with the local structural order and the corresponding energy landscape[4].

[1] F.Ebert, P.Dillmann, G.Maret, P.Keim, Rev.Sci.Instrum. 80, 083902(2009)

[2] F.Ebert, P.Keim, G.Maret, EPJE 26, 161(2008), EPJE 29, 311(2009)

[3] S.Mazoyer, F.Ebert, G.Maret and P.Keim, EPL, (2009), in print

[4] S.Mazoyer, F.Ebert, G.Maret and P.Keim, (2009) submitted

CPP 42.2 Thu 11:30 H39

Aggregation phenomena in two-dimensional systems of dipolar colloids with shielded interactions — •Anton Smessaert and Sabine H. L. Klapp — Institut für Theoretische Physik, TU Berlin, 10623, Germany

Employing Molecular Dynamics (MD) simulations we investigate aggregation phenomena and phase separation in a suspension of dielectric colloidal particles in an external field. The system is two-dimensional and the colloids are modeled as soft spheres with induced dipoles. The interaction of the dipoles is shielded in the framework of the Debye-Hückel theory [1]. For comparison we use a shifted dipole-dipole interaction supplemented by a soft sphere potential.

One part of our study is a detailed cluster analysis based on the MD simulations. Also, we employ a second order virial expansion to explore the possibility of a condensation phase transition.

Our results illustrate the influence of the interaction-range on the clustering and phase transition.

[1] S. Tsonchev, G.C. Schatz and M.A. Ratner, Chem. Phys. Lett. **400**, 221-225 (2004)

CPP 42.3 Thu 11:45 H39

Building complex arrays of colloidal particles by tuning their interactions with charged surfaces — •Christoph Hanske[1], Andreas Fery[1], and Alexander Wittemann[2] — [1]Department of Physical Chemistry II, University of Bayreuth, Universitätsstraße 30, 95440 Bayreuth, Germany — [2]Department of Physical Chemistry I, University of Bayreuth, Universitätsstraße 30, 95440 Bayreuth, Germany

Recently two-dimensional and three-dimensional mesostructures of colloidal particles have attracted the attention of material scientists due to their photonic properties. Whereas classical methods of particle deposition usually yield hexagonally ordered layers, more complex patterns are desired to vary the optical properties of the obtained materials. In order to control the interactions between particles and substrates, tailor-made colloids with a glassy core carrying a soft shell of polyelectrolyte brushes were synthesized. These particles are responsive to external stimuli like ionic strength or pH-value. Variation of these parameters does not only allow tuning the shape of the particles in solution, but also their interaction with charged surfaces. Formation of complex structures was accomplished by selective particle deposition on substrates chemically patterned by classic or lithography-free microcontact printing. In this contribution we will discuss decisive parameters governing the assembly into structured arrays which open up new avenues for building photonic materials.

CPP 42.4 Thu 12:00 H39

Role of surface charges on structure formation in confined colloidal solutions — •Stefan Grandner and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

The impact of surface charges on structural effects in confined, charged colloidal suspensions is addressed in grand-canonical Monte-Carlo simulations using a corse-grained model (DLVO). These investigations are motivated by Colloidal-Probe Atomic-Force-Microscope experiments where enhanced amplitudes of the structural forces are obtained for increased surface charges. Whereas various established approaches of the interaction between macroions and charged walls did not reproduce this behavior, we could verify it within linearized Poisson-Boltzmann theory using a modified fluid-wall interaction which takes additional wall counterions into account [1]. The main difference to former models is the wall charge dependence of the wall screening parameter yielding a non-monotonic behavior of the repulsion. Furthermore we explore the impact of charged walls on particle ordering [2], where we expect nontrivial consequences on the lateral order of the layered suspension as compared to uncharged surfaces [3].

[1] S. Grandner, Y. Zeng, R. v. Klitzing, and S. H. L. Klapp, J. Chem. Phys. **131**, 154702 (2009). [2] B. Fazelabdolabadi, J. Y. Walz, and P. R. Van Tassel, J. Phys. Chem. B **113**, 13860 (2009). [3] S. Grandner and S. H. L. Klapp, J. Chem. Phys. **129**, 244703 (2008).

CPP 42.5 Thu 12:15 H39

1, 2, and 3D Organization of Colloidal Nanoparticles — •Nicolas Pazos-Perez[1], Alexandra Schweikart[1], Adrea Fortini[2], Matthias Schmidt[2], Ramon Alvarez-Puebla[3], Luis M. Liz-Marzan[3], and Andreas Fery[1] — [1]Department of Physical Chemistry II, University of Bayreuth, Germany — [2]Department of Theoretical Physics II, University of Bayreuth, Germany — [3]Department of Physical Chemistry, University of Vigo, Spain

Colloidal crystal structures have been widely studied due to their extraordinary optical, electronic, magnetic... properties which are structure dependent. Thus, a big effort has been put in developing new methods which allow a fine control over the formation of colloidal crystals. This work presents a novel method to organize colloids into 1, 2 and 3D linear arrays in a macro scale range. This technique is based on the use of a pre-patterned polymeric stamp which provides a network of channels acting as confinement regions for the particles during the drying process. Additionally, Monte Carlo simulations were performed to study the obtained colloidal crystals morphologies. In both cases, simulation and experimental, we found a broad range of morphologies depending on the initial suspension concentration which differ from the bulk. Moreover, we demonstrate that such nanoparticulated arrays made of gold can be used for Surface Enhanced Raman Scattering (SERS) detection.

CPP 42.6 Thu 12:30 H39

Sedimentation equilibrium of colloidal platelets in an aligning magnetic field — •Matthias Schmidt[1,2] and Hendrik Reich[3] — [1]Theoretische Physik II, Universität Bayreuth, D-95440 Bayreuth, Germany — [2]H. H. Wills Physics Laboratory, University of Bristol, Royal Fort, Tyndall Avenue, Bristol BS8 1TL, United Kingdom — [3]Deutscher Wetterdienst, Frankfurter Str. 135, D-63067 Offenbach, Germany

We consider colloidal platelets under the influence of gravity and an external aligning (magnetic) field. The system is studied using a fundamental measures density functional theory for model platelets of circular shape and vanishing thickness. In the gravity-free case the bulk phase diagram exhibits paranematic-nematic phase coexistence that vanishes at an upper critical point upon increasing the strength of the aligning field. Equilibrium sedimentation profiles display a paranematic-nematic interface, that moves to smaller (larger) height upon increasing the strength of gravity (the aligning field). The density near the bottom of the system decreases upon increasing the strength of the aligning field. Using a simple model for the birefringence properties of equilibrium states, we simulate the colour variation with height, as can be observed in samples between crossed polarizers.

CPP 43: Colloids and Complex Liquids II

Time: Thursday 14:00–17:45 Location: H39

CPP 43.1 Thu 14:00 H39

Lattice Boltzmann simulations of suspensions with multiple fluid components — •Jens Harting[1,2] and Fabian Jansen[2] — [1]Dept. of Applied Physics, TU Eindhoven, Postbus 513, NL-5600MB Eindhoven — [2]Institute for Computational Physics, University of Stuttgart, Pfaffenwaldring 27, D-70569 Stuttgart

This contribution has been withdrawn.

CPP 43.2 Thu 14:15 H39

A simplified particulate model for coarse-grained hemodynamics simulations — •Florian Janoschek, Jens Harting, and Federico Toschi — Department of Applied Physics, Eindhoven University of Technology, The Netherlands

Simulation of human blood flow is a demanding task both in terms of the complexity of applicable models and 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 (RBCs) in blood plasma. A second reason is that in realistic geometries typical length scales vary over several orders of magnitude. Usual computational models either cope with this complexity by implementing only a homogenous although maybe non-Newtonian fluid or highly resolve relatively small numbers of RBCs by means of deformable meshes.

Our goal is to develop a coarse-grained and highly efficient yet still particulate model for blood that allows us to simulate up to millions of cells on current parallel supercomputers. We start with a lattice Boltzmann based simulation method for suspensions of rigid particles to account for long-range hydrodynamic interactions. Since real RBCs are not rigid we add anisotropic model potentials to cover the more complex short-range behavior of deformable cells on a phenomenological level. The benefit of the new model lies in the application to multi-scale problems in realistic geometries requiring particulate resolution in some regions and in the opportunity to investigate statistical and time dependent effects in soft particle suspensions like blood. We will present an overview of the model and its rheological properties.

CPP 43.3 Thu 14:30 H39

Changes of dynamical anisotropy characteristics of ferrofluids in a magnetic field — •Jelena Jordanovic and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Deutschland

We report a Molecular Dynamic study of the dynamical properties of a ferrofluid in equilibrium in the presence of a homogeneous magnetic field. Accordingly, the anisotropic diffusion constant as well as characteristics of the single particle motion are investigated. Experimentally[1] it was observed that diffusion in the directions perpendicular to the field is hindered compared to diffusion in the parallel direction, indicated by a $D_\perp < D_\parallel$ relation between the diffusion constants. However, an opposite relation was found in Brownian Dynamic simulations[2]. We found[3] a connection between both anisotropy characteristics, where the field strength as well as the dipole-dipole coupling strength play a key role. The mechanism behind the field-induced inversion of the diffusion constants' relation is explained from a microscopic point of view by the van Hove correlation function. Moreover, by investigating the single particle motion, we show that the inversion is accompanied by an intermediate deviation from diffusive behavior, which strongly increases with the dipole-dipole coupling strength.

[1] A. Mertelj, L. Cmok, and M. Čopič, Phys. Rev. E **79**, 041402 (2009).
[2] P. Ilg, and M. Kröger, Phys. Rev. E **72**, 031504 (2005).
[3] J. Jordanovic and S. H. L. Klapp, in preparation.

CPP 43.4 Thu 14:45 H39

Monte Carlo simulations of binary two dimensional colloidal crystals confined between planar walls — •Stefan Medina Hernando[1], Peter Virnau[2], and Kurt Binder[3] — [1]Institut für Physik, Uni Mainz, Deutschland — [2]Institut für Physik, Uni Mainz, Deutschland — [3]Institut für Physik, Uni Mainz, Deutschland

Monodisperse two dimensional systems have been studied extensively in theory, computer simulations and experiments. We extend these investigations by simulating asymmetric soft binary colloidal mixtures confined between planar walls. Two cases are presented in detail: In the commensurate case the number of rows in the system is chosen to fit properly between the walls. In the incommensurate case a mismatch is introduced which leads to the occurrence of solitons.

CPP 43.5 Thu 15:00 H39

Monte Carlo simulations of colloid-polymer mixtures in cylindrical confinement — •Alexander Winkler, Peter Virnau, and Kurt Binder — Institut für Physik, Johannes Gutenberg-Universität Mainz

We investigate the Asakura-Oosawa model in cylindrical confinement with Monte Carlo simulations. On the one hand side the system can be regarded as a model for nanopores, on the other hand the system exhibits an interesting ”phase behavior” due to its quasi-one-dimensional character. At high polymer reservoir packing fractions, the tube is either filled with liquid or gas. When we approach a ”pseudo-critical point” (at reservoir packing fractions above the critical value of the bulk) several interfaces appear and the tube contains both liquid and gas phases, which are studied by extensive Free Energy calculations.

CPP 43.6 Thu 15:15 H39

Density functional theory for a hard disc fluid on graphics cards — •Marlon Ebert — Johannes Gutenberg Universität Mainz

Investigating the rheological properties of two dimensional fluids near the freezing transition provides interesting challenges. In order to approach this problem we use density functional theory (DFT) to determine the static density correlations around one and two test particles. Since DFT calculations in more then one dimension are usually computationally expensive we resort to applying graphics cards as massively parallel computational devices, using the CUDA language. We discuss the signatures of the freezing transition in the static correlations and compare to simulation results. An extension of the static DFT method aimed at the correlation functions under shear will be discussed. From these the rheological properties of the fluid can be deduced.

15 min. break

CPP 43.7 Thu 15:45 H39

Critical Casimir Forces in Binary Colloidal Suspensions — •Olga Zvyagolskaya[1] and Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universität Stuttgart — [2]Max-Planck-Institut für Metallforschung, Stuttgart

We investigate the behavior of a dense two-dimensional colloidal system immersed in a critical binary liquid mixture of water and 2,6-lutidine in front of a plane surface. Close to the critical point critical Casimir forces arise whose sign and amplitude strongly depend on the temperature and the preferential adsorption properties of the surfaces. In our experiments we study the behavior of a binary mixture of colloidal particles with opposite preferential adsorption properties. Owing to their different Casimir interaction with the substrate, this leads to different particle motilities. As a function of the temperature, the relative particle concentrations and the preferential adsorption properties of the substrate we find a large variety of metastable structures.

CPP 43.8 Thu 16:00 H39

Airbrush-spray deposition of colloidal polymer film investigated by Grazing Incidence Small Angle X-ray Scattering — •Adeline Buffet, Gerd Herzog, Matthias Schwartzkopf, Mottakin M. Abul Kashem, Jan Perlich, Rainer Gehrke, and Stephan V. Roth — HASYLAB-DESY, Notkestr. 85, D-22607 Hamburg, Germany

Organic-based hybrid devices received strong attention from both academy and industry because of their potential for low-cost production and flexible device applications [1]. Recently, the novel technique of airbrush spray deposition was used in the fabrication of organic-based multilayer devices such solar cells [2]. This technique allows for performing rapid deposition of organic-based nanostructured layers showing high homogeneity over a large area and is thus of great interest in industrial applications. We used Grazing Incidence Small Angle X-ray Scattering (GISAXS) to investigate the structure of a colloidal nanoparticle film deposited on a flat Si-substrate by using a commercial airbrush-spray. The study shows a strong dependence of the film homogeneity on the substrate-to-spray distance and the strong influence of the solvent choice on the film lateral ordering opening a promising route to generate laterally structured templates and scaffolds for the fabrication of ultrahigh-density media. [1] G. Kaune et al., Eur. Phys. J. E 26, 73-79 (2008). [2] R. Green, et al., Appl. Phys. Lett. 92, 03330 (2008).

CPP 43.9 Thu 16:15 H39

Total internal reflection microscopy: From scattering intensity to absolute position — •Thomas Brettschneider[1], Giovanni Volpe[1,2], Laurent Helden[1], and Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [2]Max-Planck-Institut für Metallforschung, Heisenbergstraße 3, 70569 Stuttgart, Germany

Total Internal Reflection Microscopy (TIRM) is a sensitive and non-intrusive technique to measure the interaction potentials between a colloidal particle immersed in a liquid and a wall. The equilibrium distribution of the particle-wall separation distance z is sampled monitoring the intensity I scattered by the Brownian particle under evanescent illumination. From this one can determine the distance resolved interaction potential and corresponding forces with femtonewton resolution. The central point of the data analysis is the *a priori* knowledge of the relation between the measured scattering intensity I and the corresponding particle distance z. For short penetration depths of the evanescent field, it has been demonstrated that $I(z) \propto \exp(-z/\delta)$. This, however, poses considerable constraints to the experimental conditions and the range of forces where TIRM can be applied. Here, we introduce a method to experimentally determine $I(z)$ by making solely use of the distance-dependent hydrodynamic interactions between the particle and the wall. We demonstrate, that our method largely extends the range of conditions accessible with TIRM, and even allows measurements on highly reflecting gold surfaces where multiple reflections lead to large deviations from an exponential $I(z)$ relationship.

CPP 43.10 Thu 16:30 H39

Sliding of colloidal monolayers on periodic and quasiperiodic substrate potentials — •Thomas Bohlein, Jules Mikhael, and Clemens Bechinger — 2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany

Quasicrystal surfaces exhibit low friction coefficients. This anomalous property led to their consideration as coatings for tribological applications. However, the fundamental mechanisms behind this behavior are still not well understood. Here we experimentally study the sliding behavior of two dimensional colloidal crystals interacting with periodic and quasiperiodic light induced substrate potentials created by overlapping several laser beams. A precise control of the phases of the interfering beams allows us to shear the substrate potential against the crystal in any desired direction while the crystal's response is studied in real space by digital video microscopy. We study how the substrate strength, the sliding velocity and the matching of the length scales affect the sliding behavior. This allows us to identify the role of quasiperiodicity on the friction behavior which leads to a better understanding on the fundamentals of atomic fiction and superlubricity.

CPP 43.11 Thu 16:45 H39

Colloidal particles in microchannels: transport in confined geometries — •Christian Kreuter, Paul Leiderer, and Artur Erbe — University of Konstanz, Germany

Understanding of biological systems requires detailed knowledge of the transport behavior of interacting particles. Since real-life systems are typically very complex, experimentally easily accessible systems have to be investigated in order to understand the fundamental physics underlying the collective behavior. During the last years, studies of colloidal systems have become a standard approach to model and simulate real systems. In our experiments we use superparamagnetic particles and investigate the transport behavior of such interacting particles gravitationally driven through narrow channels defined by optical lithography. With this experimental system we can realize various potential shapes by crossings of channels or channels with structured walls. Furthermore we modify the transport behavior through realization of barriers perpendicular to the channel. These systems resemble, for example, transport through ion channels or electron transport in mesoscopic systems.

CPP 43.12 Thu 17:00 H39

Direct measurement of shear-induced cross-correlation of Brownian motion — •Andreas Ziehl and Christian Wagner — Universität des Saarlandes, Saarbrücken

Shear-induced cross-correlations between particle fluctuations perpendicular and along streamlines are investigated experimentally and theoretically in a linear shear flow. We used optical tweezers to localize one or two particles, each in a harmonic potential, and to detect the positions of the particles as a function of time with a high spatial precision below 8nm. These positions are recorded via a high speed camera with 15kHz resolution. In contrast to measurements in a quiescent fluid, we find that in shear flow, generated in a special designed micro fluidic device, orthogonal movements of a bead in stream- and gradient- directions are correlated and the time reversal symmetry is broken. Again in a quiescent fluid, fluctuations of two particles, separated by a few microns, are known to be anti-correlated along their connecting vector due to hydrodynamic coupling. In linear shear flow, we found a coupling process that correlates the orthogonal directions of the two particles. The correlation exhibits a minimum in time and again the time reversal symmetry is broken.

CPP 43.13 Thu 17:15 H39

Experimental accessible variables for testing a generalized fluctuation-dissipation theorem — •Jakob Mehl, Valentin Blickle, and Clemens Bechinger — 2. Physikalisches Institut, Universität Stuttgart, Germany

One cornerstone of statistical physics is the fluctuation-dissipation theorem (FDT). Generally true for all systems slightly perturbted around their equilibrium state, it connects the response of any observable to a small perturbation to equilibrium correlations involving the observable conjugated to the perturbation with respect to energy.

When leaving thermal equilibrium the FDT breaks down. Recently it was shown, that the FDT can be generalized to nonequilibrium steady states (NESS) by choosing the conjugated variable with respect to entropy. By combining colloidal particles, rotating laser tweezers, and video microscopy, we confirm experimentally the generalized FDT for a NESS. In principle the restored formulation allows infinitely many variants of the FDT. However, our experiments demonstrate, that the right choice of variables is crucial to determine the nonequilibrium response via forced fluctuations out of a NESS.

CPP 43.14 Thu 17:30 H39

Is there a Relationship between the Elongational Viscosity and the First Normal Stress Difference in Polymer Solutions? — •Stephan Gier[1], Andreas Zell[1], Salima Rafai[2], and Christian Wagner[1] — [1]Universität des Saarlandes, Saarbrücken — [2]Laboratoire de Spectrometrie Physique, Grenoble

We investigate polymer solutions in shear and elongational flow. Shear flow is created in a cone-plate-geometry of a commercial rheometer. The capillary thinning of a filament of polymer solution in the Capillary Breakup Extensional Rheometer (CaBER) serves as an elongational flow. We compare the relaxation time and the elongational viscosity measured in the CaBER with the first normal stress difference and the relaxation time from the rheometer measurements. All these four quantities depend on different fluid parameters - the viscosity of the polymer solution, the polymer concentration within the solution, and the molecular weight of the polymers - and on the shear rate (in the shear flow measurements). Nevertheless, we found that the first normal stress coefficient depends quadratically on the CaBER relaxation time. A simple model is presented that explains this relation on a phenomenological level.

CPP 44: Liquids and Ionic Liquids

Time: Thursday 9:30–10:45 Location: H45

Topical Talk CPP 44.1 Thu 9:30 H45

Glassy dynamics and charge transport in ionic liquids — •Friedrich Kremer, Joshua Sangoro, Ciprian Iacob, and Jörg Kärger — Institute of Experimental Physics I, University of Leipzig, Linnéstr. 5, 04103, Leipzig, Germany

Charge transport and glassy dynamics in 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. The dielectric spectra are dominated - on the low-frequency side - by electrode polarization effects while, for higher frequencies, charge transport in a disordered matrix is the underlying physical mechanism. 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 discussed within the framework of the concept of *dynamic glass transition driven hopping* traced back to Einstein, Einstein-Smoluchowski, and Maxwell relations. 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. It becomes possible to extract from the dielectric spectra separately the number density and the mobilities of the charge carriers and the type of their thermal activation.

CPP 44.2 Thu 10:00 H45

Determining the dielectric constant of ionic liquids from computer simulations — •Axel Arnold — ICP, Universität Stuttgart

We present a new method to reliably calculate the static dielectric constant of charged liquid matter from radial distribution functions, as they can be obtained for example from Monte Carlo or Molecular dynamics simulations. We also explain why a direct measurement of the Kirkwood factor of ionic liquids under periodic boundary conditions cannot generate physically meaningful results.

CPP 44.3 Thu 10:15 H45

Changes of the surface electronic structure of [EMIm]Tf$_2$N room temperature ionic liquid induced by copper ions — •Angela Keppler[1], Tomonori Ikari[1,2,3], Oliver Höfft[2], Markus Reinmöller[1], Wichard J. D. Beenken[1], Frank Endres[2], and Stefan Krischok[1] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany — [2]Institut für Mechanische Verfahrenstechnik, TU Clausthal, Arnold-Sommerfeld-Str. 6, 38678 Clausthal-Zellerfeld, Germany — [3]Ube National College of Technology, Department of Electrical Engineering, 2-14-1 Tokiwadai, Ube, Yamaguchi 755-8555, Japan

The influence of Cu on the surface electronic structure of [EMIm]Tf$_2$N is investigated using photoelectron spectroscopy. Cu$^+$ ions are electrochemically dissolved in [EMIm]Tf$_2$N. An enrichment of Cu in the near surface region of [EMIm]Tf$_2$N is obtained in XPS results. By comparing the copper containing IL with the neat [EMIm]Tf$_2$N a modification of the near surface chemical composition is found. The Cu induced change of the cation/anion ratio directly correlates with the amount of Cu detected by XPS. Additionally, this modifies the valence band structure, which was analysed by XPS and UPS. This modification throws some light on the origin of certain valence band structures and will be discussed on the basis of new DFT calculations. The results will be compared with available data obtained in additional experiments like Cu deposited on the liquid directly under UHV conditions and with data from other ionic liquids ([BMP]Tf$_2$N and [BMIm]dca).

CPP 44.4 Thu 10:30 H45

DFT-Analysis of Core Levels from Room-temperature Ionic Liquids — •Markus Reinmöller[1], Angela Keppler[1], Tomonori Ikari[1,2], Stefan Krischok[1], and Wichard J. D. Beenken[1] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100 565, 98684 Ilmenau, Germany — [2]Ube National College of Technology, Department of Electrical Engineering, 2-14-1 Tokiwadai, Ube, Yamaguchi 755-8555, Japan

We performed quantum-chemical calculations by means of density functional theory (DFT) on single ion pairs from imidazolium-based ionic liquids. Thereby we varied the alkyl-chains attached to the imidazolium cation, e.g. from ethyl to octyl at the 1-position, as well as the anion from small like Cl$^-$, Br$^-$ and BF$_4{}^-$ to more complex like Tf$_2$N$^-$.

By means of the calculated density of states (DOS) projected to the contributions of single atoms, we could directly correlate our theoretical results to experimental XPS data [1], in particular the chemical shifts and splittings of the carbon and nitrogen 1s core level emission.

[1] T. Ikari, A. Keppler, M. Reinmöller, W. J. D. Beenken, S. Krischok, M. Marschewski, W. Maus-Friedrichs, O. Höfft, F. Endres, submitted to e-Journal of Surface Science and Nanotechnology, 2009.

CPP 45: Focus: Charge Effects in Soft and Biological Matter I (jointly with BP)

Time: Thursday 11:00–12:45 Location: H45

Invited Talk CPP 45.1 Thu 11:00 H45

Charge effects in RNA folding — •Lois Pollack — Cornell University, Ithaca, NY USA

Because nucleic acid backbones possess such a high negative charge, interactions with positively charged ions (or larger charged molecules) are critically important to the biophysics of both RNA and DNA. Our studies of the earliest events in RNA folding highlight the importance of electrostatic interactions to this conformational change. Complementary x-ray scattering experiments on short nucleic acid duplexes have elucidated the spatial distribution of condensed counterions, as well as ion-induced interactions between duplexes. Interactions between these helices can be tuned from repulsive to attractive by varying counterion charge and concentration. Interesting differences between RNA and DNA are revealed by these measurements.

CPP 45.2 Thu 11:30 H45

Dielectrophoresis: a new tool for continuous DNA/protein interaction studies — •Martina Everwand, Dario Anselmetti, and Jan Regtmeier — Experimental Biophysics & Applied Nanoscience, Bielefeld University, Universitätsstr. 25, 33615 Bielefeld

The investigation of DNA-protein interactions is of central interest in today‘s proteomic research like for the metabolic pathway analysis. Here, a novel microfluidic device is presented, which allows efficient separation of protein-complexed DNA from native DNA strands in continuous mode.

The Lab-on-chip device consists of a 3D-structured microfluidic channel network incorporating an integrated barrier with nanometer dimension, that allows for electrodeless dielectrophoresis of DNA-protein complexes.

For the first time, we demonstrate that differently sized DNA fragments as well as DNA/protein and DNA/antibiotics complexes can be continuously separated from unbound DNA at a nano-microfluidic interface.

Invited Talk CPP 45.3 Thu 11:45 H45

Origin of the electrophoretic force on DNA in solid-state nanopores — •Serge G. Lemay — MESA+ Institute for Nanotechnology, University of Twente

Despite gel electrophoresis being one of the main workhorses of molecular biology, the physics of polyelectrolyte electrophoresis in a strongly confined environment remains poorly understood. Theory indicates that forces in electrophoresis result from interplay between ionic screening and hydrodynamics, but these ideas could so far be addressed only indirectly by experiments based on macroscopic porous gels. I will present a direct experimental based on measuring the electrophoretic force on a single DNA molecule threading through a solid-state nanopore as a function of pore size. The stall force gradually decreases on increasing the nanopore diameter from 6 to 90 nm, inconsistent with expectations from simple electrostatics and strikingly demonstrating the influence of the hydrodynamic environment. We model this process by applying the coupled Poisson-Boltzmann and Stokes equations in the nanopore geometry and find good agreement with the experimental results.

CPP 45.4 Thu 12:15 H45

DNA Translocation through Nanopores: What is the role of dielectric permittivity? — •Stefan Kesselheim[1], Marcello Sega[2], Mehmet Süzen[3], and Christian Holm[1] — [1]Institut für Computerphysik, Universität Stuttgart — [2]Department of Physics and INFN, University of Trento — [3]Institute of Photonic Sciences, Castelldefels (Barcelona), Spain

We investigate the free energy barrier of a single DNA molecule filed through a synthetic nanopore. We employ a recently developed algorithm (ICC*) that allows to take into account the dielectric contrast at the membrane/solute interface in coarse-grained molecular dynamics simulations. The investigations show the crucial contribution of dielectric mismatch to the translocation free energy barrier. We show that for low ionic strength and DNA fragments up to 100 bp the dielectric boundary forces dominate over the entropic contribution caused by DNA flexibility.

CPP 45.5 Thu 12:30 H45

DNA: charge localisation and pathogenesis. — Chi-Tin Shih[1], Yun-Yin Cheng[1], •Stephen A Wells[2], Rudolf A Römer[2], and Ching Ling[3] — [1]Department of Physics, Tunghai University, 40704 Taichung, Taiwan and The National Center for Theoretical Sciences, 30013 Hsinchu, Taiwan — [2]Department of Physics and Centre for Scientific Computing, University of Warwick, Gibbet Hill Road, Coventry, CV4 7AL, UK — [3]Department of Physics, Chung-Yuan Christian University, Chung-Li, Taiwan

We present results from transfer-matrix modelling of charge localisation and transport in DNA sequences, using tight-binding models at several levels of detail. With parallel computing resources we are able to examine the variation in local charge-transport properties along sequences of hundreds of thousands of base pairs, covering entire genes. This has allowed us to survey large numbers of human genes for which databases of pathogenic mutations exist; we consider both cancer-related genes and those associated with other forms of genetic disorder.

Examining the correlations between charge transport (CT) properties and the sites where pathogenic mutations are observed, we find a statistically significant correlation between pathogenesis and below-average changes in CT properties. We discuss the interpretation of our results in the context of DNA physics and chemistry, and of possible cellular mechanisms for DNA damage avoidance, detection and repair.

CPP 46: Focus: Charge Effects in Soft and Biological Matter II (jointly with BP)

Time: Thursday 14:00–17:45 Location: H37

Invited Talk CPP 46.1 Thu 14:00 H37

Electrostatic effects on depletion forces — •Roberto Piazza[1], Stefano Buzzaccaro[1], Jader Colombo[2], and Alberto Parola[2] — [1]Dipartimento CMIC, Politecnico di Milano, Milano (Italy) — [2]Dipartimento di Fisica e Matematica, Università dell'Insubria, Como (Italy)

Short-ranged depletion forces give rise to a phase behavior which is totally foreign to simple molecular systems, allowing to investigate new scenarios of noticeable interest for condensed matter physics. Yet, so far, most experimental and theoretical efforts have concentrated on depletion effects induced by an ideal agent.

Here, conversely, we focus on systems where strong electrostatic coupling is present. After reviewing some recent results we have obtained by sedimentation measurements on a model system of "sticky" hard-spheres, where depletion forces are induced by nonionic surfactants, we shall present novel results pointing out the dramatic effects that the presence of a self-interacting depletant may bring in. In particular, we shall show that electrostatic repulsive forces between the depletant yield a strong increase of depletion effects, scaling with the Debye-Hückel screening length. Conversely, competitive electrostatic forces between the colloidal particles hinder, and may even totally quench depletion-induced phase separation. The observed effects are fairly well accounted for by a theoretical analysis, based on liquid-state theory, of the structural properties of the two-components (colloids + surfactant micelles) fluid.

CPP 46.2 Thu 14:30 H37

Interaction of Proteins with Spherical Polyelectrolyte Brushes — •Katja Henzler[1,2], Alexander Wittemann[1], Björn Haupt[1,2], Oleg Borisov[3], and Matthias Ballauff[2] — [1]Universität Bayreuth, Physikalische Chemie I; Universitätstr. 30, 95440 Bayreuth, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie; Hahn-Meitner-Platz 1; 14109 Berlin, Germany — [3]Institut pluridisciplinaire de Recherche sur l' Environement et les Materiaux, UMR 5254, CNRS/UPPA, 64053 Pau, France

Spherical polyelectrolyte brushes (SPB) are a novel class of carrier particles for the immobilization of proteins.[1] A high uptake of proteins can be achieved if the ionic strength is low, while both compounds carry an overall negative charge.[1] No adsorption takes place at higher ionic strength. The main driving force for the adsorption is the counterion release force. Counterions from the brush layer are released and the free energy of the system will be decreased. The thermodynamic of the described adsorption process can be investigated by isothermal titration calorimetry (ITC).[2] This method allows us to determine the adsorption isotherm together with the adsorption enthalpy and entropy. We demonstrated that the adsorption of β-lactoglobulin (BLG) onto the SPB is driven by a strong gain of entropy i.e. by the postulated uptake mechanism of the counterion release force. This is the first direct proof for the counterion release force.

Literature: [1] Wittemann, A.; Ballauff, M. Phys. Chem. Chem. Phys. 2006, 8, 5269. [2] Henzler, K.; Haupt, B.; Lauterbach, K.; Wittemann, A.; Borisov, O.; Ballauff, M. in preparation.

CPP 46.3 Thu 14:45 H37

On the Question of Universality of Charge Induced Reentrant Condensation of Proteins — •Fajun Zhang[1], Benjamin Heck[1], Marcell Wolf[1], Luca Ianeselli[1], Michael Ziller[1], Maximilian W. A. Skoda[2], Robert M. J. Jacobs[3], Oliver Kohlbacher[4], Sophie Weggler[5], Andreas Hildbrandt[5], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — [2]ISIS, Rutherford Appleton Laboratory, UK — [3]Department of Chemistry, CRL, University of Oxford, UK — [4]Zentrum für Bioinformatik Tübingen, Tübingen, Germany — [5]Zentrum für Bioinformatik Saar, Saarbrücken, Germany

The effective interactions and phase behavior of protein solutions under strong electrostatic coupling conditions are a challenge to our understanding due to the complex charge pattern and irregular geometry of protein surfaces, which distinguishes them from related systems such as DNA or conventional colloids. In this work, we discuss the question of the universality of the reentrant condensation (RC) of proteins in solution induced by multivalent counterions, i.e. redissolution upon adding further salts after phase separation, as recently discovered [1]. The discussion is based on a systematic investigation of five different proteins with different charge patterns with five typical multivalent counterions. Zeta potential measurements confirm the effective charge inversion of proteins in the reentrant regime via binding of multivalent counterions. [1] F. Zhang, et al., Phys. Rev. Lett. 2008, 101, 148101.

CPP 46.4 Thu 15:00 H37

Effective charge of globular proteins and denrimers — Ute Böhme and •Ulrich Scheler — Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, 01069 Dresden

The density of charges on macromolecules is usually so high, that the thermal energy of the respective counterions is insufficient to escape the electric field generated from the charges on the macromolecule. Therefore a fraction of counterions condenses on the macromolecule, lowering the effective charge of the. The combination of diffusion and electrophoresis NMR provides an umambiquous possibility for the experimental determination of the effective charge, which is in good agreement with molecular simulations [1, 2]. This approach has been applied to linear poylelectrolytes as well as proteins and other globular molecules [3]. PAMAM dendrimers exhibit only two types of chargeable groups, therefore counterion condensation can easily be quantified, where the degree of protonation of the amino groups is inferred from proton NMR spectra. At low generations the fraction of condensed counterions increases with increasing molecular weight to level at about 70%. [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] Ute Böhme, Ulrich Scheler Chemical Physics Letters 435, (2007), 342

CPP 46.5 Thu 15:15 H37

Charge effects in protein diffusion — •Marcus Hennig[1,2], Felix Roosen-Runge[2], Fajun Zhang[2], Tilo Seydel[1], and Frank Schreiber[2] — [1]Institut Laue-Langevin, Grenoble, France — [2]Institut für Angewandte Physik, Universität Tübingen, Germany

Proteins in solution form highly monodisperse colloidal suspensions. Hence, protein solutions are of fundamental interest in a context of soft matter science. A distinguishing feature to simple colloidal systems is the inhomogeneous surface charge distribution of proteins, which is assumed to have a fundamental biological relevance in controlling for instance aggregation phenomena and docking processes. In their native environment proteins are embedded in a crowded solution of various macromolecules and salt ions. These salt ions are crucial for the understanding of the effective interactions of proteins and the dynamics. We study the self-diffusion of the model globular protein Bovine Serum Albumin in aqueous solutions with different salt concentrations by quasi-elastic neutron scattering performed at selected temperatures and in high protein concentrations. Furthermore, by using spin-echo spectroscopy we investigate the collective diffusion behavior. We found that trivalent salts, particularly yttrium chloride, have a pronounced effect on the self and collective diffusion on a nanosecond time scale. Whereas monovalent and divalent salts, such as sodium chloride and calcium chloride, exhibit little or no effect, we observe that the diffusion decreases nearly 50% for a 19mM yttrium chloride concentration.

15 min. break

Invited Talk CPP 46.6 Thu 15:45 H37

In-silico simulation of reentrant protein condensation with highly valent counterions — Sophie Weggler[1], Michael Ziller[2], Fajun Zhang[2], Frank Schreiber[2], Oliver Kohlbacher[3], and •Andreas Hildebrandt[1] — [1]Center for Bioinformatics, Bld. E 2.1, Saarland University, 66123 Saarbrücken, Germany — [2]Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — [3]Zentrum für Bioinformatik Tübingen, Sand 14, 72076 Tübingen, Germany

Recently, it has been shown experimentally that negatively charged globular proteins in solution undergo a condensation upon adding trivalent counterions between two critical concentrations C^* and C^{**}, $C^* < C^{**}$. This reentrant condensation had previously been observed for DNA and suitable colloidal systems, where the phenomenon is well-understood theoretically, but not for proteins: while the former systems can be well approximated by simple geometries and constant surface charge distributions, proteins feature complex charge patterns on their surface and can occur in diverse geometrical arrangements.

Consequently, the mechanism behind reentrant protein condensation differs from that behind reentrant DNA condensation and can be explained by short-ranged electrostatic interactions between multivalent cations and acidic residues of the protein.

In my talk, I will present a theoretical model for reentrant protein condensation and will introduce a Monte Carlo technique for its numerical simulation.

CPP 46.7 Thu 16:15 H37

Oligolamellar Lipid Layers Under Load: A Model For Artificial Implants — •Martin Kreuzer[1], Reiner Dahint[1], and Roland Steitz[2] — [1]Universität Heidelberg, Physikalisch Chemisches Institut, 69120 Berlin, Germany — [2]Helmholtz-Zentrum Berlin GmbH, 14109 Berlin, Germany

The mechanisms and physicochemical parameters to reduce friction in a natural joint are not yet clear and subject of controversial discussions. We represented the biological interface by a suitable model system and employed Neutron Reflectivity for studying the relevant structural features on the molecular scale. The model interface consisted of a lipid covered silicon disc measured against a model synovial fluid at elevated hydrostatic pressure. Measurements in a pressure cell against D2O showed, that the as-prepared lipid coating remained stable on the substrate up to a hydrostatic pressure of 900bar when the lipid molecules were in their gel-like $P\beta^*$ phase. However, the lipid main phase transition from the gel to fluid-like $L\alpha$ phase at 450 bar and 38°C lead to a loss of most of the lipid bilayers and only one double layer remained on the substrate. Measurements against the model synovial fluid (3mg/ml hyaluronic acid in D2O) showed that the lipid multilayer coatings remained stable on the substrate at 450 bar and 38°C, where formerly the phase transition into the fluid-like $L\alpha$ phase occurred. Beside that, a pronounced swelling of the oligo-lamellar films was observed. Therefore, we conclude that the synovial fluid not only plays an important role in the reduction of friction in the human joint, but also significantly stabilizes the lipid multilayer coating.

CPP 46.8 Thu 16:30 H37

Ion specificity and the Jones-Ray effect at liquid-liquid interfaces — •Markus Bier — Max-Planck-Institut f. Metallforschung, Heisenbergstr. 3, 70569 Stuttgart, Germany

The solvation shells around ions in solution are one of the key features which determine, e.g., the kinetics of electrochemical reactions and the charge transport across ion channels in biological membranes. Ion specificity of certain properties is, to a large extent, brought about by a variation of the structure or the stability of the solvation shell when considering different types of ions. In the present contribution the interfacial tension between two immiscible liquids as a function of the ionic strength is studied theoretically. For large ionic strengths the well-known linear behaviour is found, which is related to a finite size of the solvation shells. For small ionic strengths a decrease with the negative square root occurs due to an unequal partitioning of ions near the interface, which is induced by a difference of the solvation free energy contrasts between the two liquids. The crossover ionic strength between both regimes turns out to be strongly ion specific. A minimum of the interfacial tension can occur close to the crossover ionic strength, similar to the Jones-Ray effect of the electrolyte-air surface. The theoretical results are compared with experimental data and the relation to the limiting case of an electrolyte-air surface is discussed. It is argued that the dependence of the liquid-liquid interfacial tension on the ionic strength could serve as a sensitive probe to study solvation shells of various ions in various liquids.

CPP 46.9 Thu 16:45 H37

Three-layer piezoelectrets from fluoroethylenepropylene (FEP) copolymer films: Arrangement, preparation and characterization — •Peng Fang[1], Feipeng Wang[1], Werner Wirges[1], Heitor Cury Basso[2], and Reimund Gerhard[1] — [1]Applied Condensed-Matter Physics, Department of Physics and Astronomy, Faculty of Science, University of Potsdam, Potsdam-Golm, Germany — [2]Department of Electrical Engineering, São Carlos School of Engineering, University of São Paulo, São Carlos - SP, Brazil

Piezoelectrets are very useful transducer materials for electromechanical and electroacoustical sensors and actuators. A new process for the preparation of three-layer FEP-sandwich piezoelectrets is introduced. The samples are prepared from commercial FEP films by means of simple procedures such as laser cutting, laser bonding, electrode evaporation and high-field poling. The resulting dielectric-resonance spectrum demonstrates the piezoelectricity of the FEP sandwich. A DC poling voltage of around -4 kV is sufficient to achieve piezoelectric d33 coefficient as high as 40 to 50 pC/N. After a continuous dynamic measurement of d33 over 5000 cycles (around 1 day), samples still retain 90% of their initial piezoelectricity. Higher measuring frequencies lead to a decrease of d33. At 100 Hz, d33 is 70% of the value at 2 Hz. Samples charged at elevated temperatures show much better thermal stability of d33. No obvious decay of d33 is found on samples charged at 130 degree C after one-hour storage at 120 degree C. Samples retain more than half of their initial piezoelectricity after a thermal treatment at 140 degree C and are still piezoelectric at 160 degree C.

CPP 46.10 Thu 17:00 H37

The conformation of poly(styrene sulfonate) layers physisorbed from salt solutions of different concentration studied on two different length scales: superposition of electrostatic and steric forces — •Stephan Block and Christiane A. Helm — Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Str. 6, D-17489 Greifswald, Germany

AFM is used to measure the surface forces and to image sodium poly(styrene sulfonate) (PSS) layers physisorbed from NaCl solutions with an ionic strength ranging between 0 M and 1 M NaCl. Colloidal probe tapping mode imaging shows that domains of PSS brushes coexist with flatly adsorbed PSS. The brush area fraction increases with rising degree of polymerization and NaCl concentration in the adsorption solution. Colloidal probe technique reveals that the surface forces are a superposition of steric and electrostatic forces, their respective contribution is determined by the brush area fraction. Interestingly, the internal properties of the brush domains (i.e. brush thickness and average chain distance) are independent on the adsorption salt concentration and depend only on the degree of polymerization and (for the brush thickness) on the surrounding salt concentration. Using these complementary techniques we derive the scaling laws for the average chain distance and the brush thickness and area fraction. Thereby it is possible to form PSS brushes with the desired properties (brush thickness between 20 and 400 nm, brush area fraction between zero and full surface coverage) and hence to control the range and magnitude of the surface forces by choosing the appropriate preparation conditions.

CPP 46.11 Thu 17:15 H37

Changes of the Molecular Structure in Supported Polyelectrolyte Multilayers under Mechanical Stress — •Johannes Früh[1], Mareike Kiel[1,2], Ralf Köhler[1,3], and Rumen Krastev[1,4] — [1]Max Plank Institut für Kolloid- und Grenzflächenforschung, 14424 Potsdam, Germany — [2]Uni Potsdam, 14476 Potsdam, Germany — [3]Helmholtz-Zentrum Berlin, 14109 Berlin, Germany — [4]NMI an der Universität Tübingen, 72770 Reutlingen, Germany

Polyelectrolyte multilayers (PEM) are extensively applied in contemporary technique. They are composed of oppositely charged polymers. The build-up process is based on the electrostatic interactions between the interface and the polymer molecules. Application of lateral stress on PEM changes the molecular conformation and the orientation of the polymers, and the electrostatic interactions between them. This leads to changes in the interfacial properties of the PEM coatings. The pyrene fluorescence is a tool to study the molecular coiling and polarity in PEM. We used this to follow the changes in the molecular structure of PEM prepared from pyrene labelled poly-styrene sulphonate and poly-(diallyldimethylammonium) chloride deposited on sheets of PDMS. We found that PEM undergo a plastic deformation under mechanical stretching. The polymer molecules organised in PEM experience a transition from coiled to decoiled state. The deformation strongly depends on the salt concentration of the solution from which the PEM are prepared, respectively on the molecular coiling and electrostatic interactions.

CPP 46.12 Thu 17:30 H37

About the interfacial behaviour of PEM films of different charge density — •Ralf Köhler[1,2], Ingo Dönch[1], Patrick Ott[3], André Laschewsky[3], Andreas Fery[4], and Rumen Krastev[1,5] — [1]MPI of Colloids and Interfaces, 14424 Potsdam — [2]Helmholtz Centre Berlin for Materials and Energy, 14109 Berlin — [3]University of Potsdam, 14476 Potsdam — [4]University of Bayreuth, 95440 Bayreuth — [5]NMI at the University of Tübingen, 72770 Reutlingen, Germany

Polyelectrolyte Multilayers (PEM) consist in complexed layers of organic polyions of opposite charge build-up on solid substrate by layer-by-layer deposition. Although PEM materials are studied since more than a decade, the interplay of internal interactions and structure is still far from being understood.

We investigate the internal structure of PEM by means of swelling experiments, i.e. an internal mechanical stress is induced into PEM by uptake of solvent molecules from adjacent solvent vapour (H2O) of varying saturation. 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.

Three different PEM systems made from PSS/PDDA (1) are investigated; each containing a derivative of the polycation PDDA of 75, 89, or 100% charge density, also the number of adsorbed layers is varied.

It shows that the swelling characteristics changes continuously with the initial film thickness indicating internal transitions of structure and swelling. (1) poly-styrene sulphonate/ poly-diallyldimethyl ammonium

CPP 47: Focus: Charge Effects in Soft and Biological Matter III (jointly with BP)

Time: Friday 10:15–12:00 Location: H45

Invited Talk CPP 47.1 Fri 10:15 H45

Charge inversion in macromolecular systems — •Christian Holm — Institut für Computerphysik, Universität Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart, Germany

We discuss our current understanding of the phenomenon of charge inversion in macromolecular systems, based on simulational results in recent years. In this approach the solvent has been incorporated only as an implicit dielectric background, whereas all charges and salt ions are treated explicitly. We will also discuss our recent work on modelling electrophoresis of charged polymers within a coarse grained approach, where the solvent degrees of freedom have been modelled using a Lattice-Boltzmann algorithm.

[1] R. Messina, C. Holm, K. Kremer,*Ground state of two unlike charged colloids: an analogy with ionic bonding*, Euro. Phys. Lett., **51**, 461 (2000).

[2] O. Lenz, C. Holm, *Simulation of charge reversal in salty environments: Giant overcharging?*, Euro. Phys. J. E **26**, 191-195 (2008).

[3] K. Grass, C. Holm *Mesoscale modelling of polyelectrolyte electrophoresis*, Faraday Discuss. **144**, 57-70 (2010).

CPP 47.2 Fri 10:45 H45

Counterion condensation and effective charge of linear and globular macromolecules — Ute Böhme and •Ulrich Scheler — Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, 01069 Dresden

The charge density on charged macromolecules is usually so high, that the thermal energy of the respective counterions is insufficient to escape the electric field generated from the charges on the macromolecule. Therefore a fraction of counterions condenses on the macromolecule, lowering the effective charge of the macromolecule The combination of diffusion and electrophoresis NMR provides an umambiquous possibility for the experimental determination of the effective charge, which is in good agreement with molecular simulations [1, 2]. This approach has been applied to flexible and stiff polyelectrolytes as well as proteins and other globular molecules [5]. Because PAMAM dendrimers exhibit only two types of chargeable groups, counterion condensation can easily be quantified, where the degree of protonation of the amino groups is inferred from proton NMR spectra. The fraction of condensed counterions increases with increasing molecular weight to level at about 70%. The effect of the variation of the solvent properties is studied with variation of the ionic strength and the dielectric constant of the solution.

[1] K. Grass, U. Böhme, U. Scheler, H. Cottet, C. Holm, Physical Review Letters 100, (2008) 096104 [2] U. Scheler, Current opinion in Colloid & Interface Science, 14 (2009), 212 [3] U. Böhme, U.Scheler, Coll. & Surf.A,, 222, (2003), 35

CPP 47.3 Fri 11:00 H45

Detection of multilayer formation of charged macromolecules by field-effect devices: from experiment to theory — •Andrey Cherstvy[1], Mariam Abouzar[2], and Arshak Poghossian[2] — [1]IFF-2, FZ Jülich, Germany — [2]IBN-2, FZ Jülich, Germany

Field-effect based semiconductor devices for label-free detection of adsorption of charged macromolecules are widely used for biosensor applications. The quantitative understanding of signals measured is however still missing in many cases. We use a capacitive electrolyte-insulator field-effect device for electrical detection of layer-by-layer adsorption of oppositely charged polyelectrolyte PE PSS/PAH chains onto the sensor surface [1]. We measure the thickness of PE layers formed as well as the changes in morphology and wetability of the modified sensor surface. We also study the effects of ionic strength on the sensor signal detected upon PE multilayer formation. We observe progressively decaying oscillations of the sensor potential upon repetitive PE adsorption. To analyze these zig-zag variations, we develop a theoretical model that accounts for the Debye screening by mobile ions within the PE layer. The model predicts that potential oscillations monitored by the sensor originate from the sign and the charge density of last PE layer. These variations depend strongly on bulk electrolyte concentration and physical parameters of PE multilayers. At lower salt, the oscillations predicted are much larger and more persistent with number of PE layers deposited. The magnitude and decay length of oscillations are in good agreement with experimental observations.

[1] A. G. Cherstvy et al., submitted to J. Phys. Chem. B.

CPP 47.4 Fri 11:15 H45

Electrostatic interactions control the permeability of biological hydrogel filters — •Oliver Lieleg[1,3], Lucy Colwell[1,2], Regina Baumgärtel[1,3], Ioana Vladescu[1], Michael Brenner[2], Andreas Bausch[3], and Katharina Ribbeck[1] — [1]FAS Center for Systems Biology, Harvard University, Cambridge, USA — [2]School of Engineering and Applied Sciences, Harvard University, Cambridge, USA — [3]Lehrstuhl für Zellbiophysik E27, Technische Universität München, Germany

The controlled exchange of molecules between biological entities (organelles, cells, or organisms) and their environment is critical for life. Biological hydrogels appear well suited to achieve such selective exchange: A hydrogel within the nuclear pore controls the passage of material between the nucleus and the cytoplasm. Mucus hydrogels lining the uterus, the stomach or the lung allow us to expel ingested particles and defend the cells beneath from a variety of pathogens. Extracellular matrix hydrogels in the connective tissue regulate the distribution of growth factors, proteins or drugs. Although hydrogel based filters are integral parts of biology, clear concepts of how their barrier function is controlled on a microscopic level are missing. Here, we discuss three biological hydrogels which differ in terms of their composition and biological function, but nevertheless seem to share a common physical design principle that regulates their microscopic barrier function: We demonstrate that particle translocation in these hydrogels is based on electrostatic interactions between diffusing particles and the hydrogel polymers rather than size exclusion effects.

CPP 47.5 Fri 11:30 H45

Diffusion and charge transport in ionic liquids: the role of ion-ion interactions — •Joshua Sangoro, Ciprian Iacob, Jörg Kärger, and Friedrich Kremer — Institute of Experimental Physics I, University of Leipzig, Linnéstr. 5, 04103, Leipzig

Self-diffusion in a variety of glass-forming ionic liquids (ILs) are investigated in a wide frequency and temperature range by means of Broadband Dielectric Spectroscopy(BDS) and Pulsed Field Gradient Nuclear Magnetic Resonance (PFG NMR). It is experimentally shown that in the time-scale characterising the cross-over from sub-diffusive to diffusive ion dynamics, the hopping lengths are of the order of molecular diameters determined from quantum-chemical calculations. This provides a direct means - via Einstein-Smoluchowski relation - to determine diffusion coefficients by BDS over more than 8 decades unambiguously and in quantitative agreement with independent PFG NMR measurements. Unprecedented possibilities in the study of charge transport and dynamic glass transition are thus opened.

CPP 47.6 Fri 11:45 H45

Collapse of highly charged polyelectrolytes triggered by attractive dipole-dipole interactions — •Andrey Cherstvy — IFF-2, FZ Juelich

We study the collapse of flexible highly charged polyelectrolyte PE chains induced by attractive dipole-dipole interactions [1]. The latter emerge due to formation of dipoles between the chain monomers and counterions condensed on PE from solution. Using the statistics of slightly perturbed Gaussian polymers, we obtain the scaling relations for PE dimensions as a function of PE charge density in the limit of compacting chains. The results are in good agreement with the outcomes of MD simulations of collapse of flexible PEs with explicit counterions. Then, we analyze the results of MD simulations for complex formation by two highly charged PEs carrying opposite charges. We use the scaling arguments based on the picture of complexation of electrostatic blobs to rationalize the size of complexes of the two chains in the collapsed state. We also analyze PE linear charge densities required for the onset onto collapse. [1] A. Cherstvy, submitted to JPCB.

CPP 48: Colloids and Complex Liquids III

Time: Friday 10:15–11:30 Location: H39

Topical Talk CPP 48.1 Fri 10:15 H39

Structural arrangement and picosecond dynamics of phospholipids in colloidal systems — •Tobias Unruh, Sebastian Busch, and Martin Schmiele — Technische Universität München, Forschungsneutronenquelle Heinz Maier-Leibnitz and Physik Department E13, 85747 Garching

Phospholipids (PL) are extensively studied for decades mainly because they form the dominant constituent of biological membrans. Furthermore, PL are widely used for stabilization of dispersions, solubilization of hardly soluble substances, and as liposomes and vesicles in food and pharmaceutical industry. However, only little is known so far about the molecular arrangement and dynamics of the stabilizing PL layers in native, technological relevant nanodispersions.

In this talk it will be demonstrated that it is possible to gain detailed structural information about the PL stabilizer layer in nanodispersions by combining X-ray and neutron small angle scattering studies with ab initio calculations of the complex scattering patterns. The mobility of PL molecules in the liquid crystalline phase but also in the stabilizer layer of nanodispersions was studied by quasi elastic neutron scattering. Using this method it could be observed that on a picosecond time scale PL molecules perform rather a directed flow-like (collective) motion than a random walk-like diffusive motion. This observation is essential for the understanding of transport processes in biological membranes over distances in the lower nanometer range and is found to be in excellent agreement to recent molecular dynamics simulations.

CPP 48.2 Fri 10:45 H39

On the diffusion of circular domains on a spherical vesicle — •Saeedeh Aliaskarisohi and Thomas.M Fischer — Institut fuer Experimentalphysik, Universitaet Bayreuth, 95440 Bayreuth, Germany

Tracking the motion of lipid domains on a vesicle is a rheological technique allowing the measurement of 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. 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. Experiments on domains in vesicles of a mixture of dioleoyl phosphatidylcholine (DOPC),dipalmytoylphosphatidylcholin(DPPC),and cholesterol(Chol) exhibit diffusion that is entirely controlled by dissipation into the water. The diffusion is suppresed compared to the diffusion of isolated domains in a flat membrane due to confinement to the curved vesicle and by hydrodynamic interactions between the domains. Effects of surface shear viscosity can be neglected.

CPP 48.3 Fri 11:00 H39

Flow dynamics in anisotropic quasi two-dimensional liquids — •Kirsten Harth, Alexey Eremin, and Ralf Stannarius — Otto-von-Guericke-Universität Magdeburg, Institut für Experimentalphysik

Thin free-standing films of tilted thermotropic smectic phases represent the simplest quasi two-dimensional anisotropic liquids. These mesophases possess a layered structure where mesogens can flow liquid-like within the layer plane. Coupling between orientation and flow fields within the film are unique to such systems.

We investigate the relaxation of specially prepared initial non-equilibrium states in three particularly simple geometries. Experimental observations are made with a polarising microscope. For a theoretical analysis, the dynamic equations - the anisotropic incompressible Navier-Stokes equation and the torque balance equation - are solved using standard finite element methods. We observe two essentially different types of stick-slip motion around central vortices (defects of the director field with topological strengths ±1). It is demonstrated that macroscopic flow patterns are generated by the inhomogeneous director relaxation, and vice versa.

We show that a neglection flow coupling in the description of relaxation processes leads to large quantitative and even qualitative errors. Comparison of experiments and simulations yields information on viscosity coefficients and elastic constants of the mesophase.

CPP 48.4 Fri 11:15 H39

Coarsening and Structure analysis of thermotropic liquid crystal foams — •Torsten Trittel, Thomas John, and Ralf Stannarius — Otto-von-Guericke-Universität Magdeburg

Foams made from surfactant solutions (aqueous foams) are well investigated and understood, but so far, there has been no report of properties of thermotropic liquid crystal (LC) foams, which can be made from pure smectic material. This type of foams has distinct microscopic properties, compared to soap foams. Owing to their inner structure, they are much more stable than aqueous foams. In our experiments, we investigate two-dimensional foams, made from smectic A LC-material, by means of digital image analysis. We focus on the temporal evolution (ageing) and describe quantitatively the asymptotic behaviour. Fundamental scaling laws are derived for the mean cellarea, number of cells, distribution of n-polygons, Aboav-Weaire-law, etc.

CPP 49: Elastomers and Gels

Time: Friday 10:15–12:15 Location: H48

CPP 49.1 Fri 10:15 H48

Reinforced elastomers: Measurement of the strain at various scales and mesoscale modelling of reinforcement and non linear properties. — •Paul Sotta[1], Stéphane Dupres[2], Samy Merabia[3], Pierre-Antoine Albouy[2], and Didier Long[1] — [1]Laboratoire Polymères et Matériaux Avancés CNRS/Rhodia, Saint-Fons, France — [2]Laboratoire de Physique des Solides, CNRS/Université Paris 11, Orsay, France — [3]Laboratoire de Physique de la Matière Condensée et Nanostructures, Université de Lyon, France

Combining mechanics, 2H NMR on stretched samples and measurement of strain-induced crystallization, we have measured the strain at various scales in polyisoprene elastomers reinforced with carbon black. We have shown that local strain inhomogeneity is more pronounced in the presence of more reinforcing carbon black grades [S. Dupres et al., Macromolecules, 2009, 42, 2634]. Related to these and other experimental results, we have developed a new mesoscale modelling of reinforced elastomers in which the glass transition temperature shift of the elastomer matrix close to fillers is implemented. The model gives a unified picture of an ensemble of complex phenomena in both the linear and nonlinear regimes of reinforced elastomers: reinforcement over a large temperature range, Payne and Mullins effects, plasticity [S. Merabia et al., Macromolecules, 2008, 41, 8252; S. Merabia et al., submitted to J. Polym. Sci. B, Polym. Phys., 2009].

CPP 49.2 Fri 10:30 H48

Caloric and optical studies of the influence of fumed silica nanoparticles on the cross-linking of polydimethylsiloxane — •Ulrich Müller, Bartosz Zielinski, Martine Philipp, Roland Sanctuary, and Jan Kristian Krüger — Université du Luxembourg, Laboratoire de Physique des Matériaux, Campus Limpertsberg, 162a avenue de la Faiencerie, L-1511 Luxembourg

Silicone rubbers based on polydimethlysiloxane (PDMS) are synthetic elastomers with outstanding properties such as chemical resistance, wide range temperature resistance, biocompatibility etc. Furthermore since the late 80s there is an increasing interest in improving the silicone rubbers properties by the introduction of fumed silica particles. Hydrogen groups on the particle*s surface are known to exhibit strong interaction with the siloxane backbone of PDMS. But there are only a few studies concerning the influence of these interactions on property evolution during the cross-linking process. We showcase that fumed silica nanoparticles have a profound impact on the cross-linking of a room temperature vulcanized silicone rubber as evidenced by caloric and optical studies. Another point of view on the cross-linking process is given by the first-time implementation of temperature modulated refractometry (TMR) that allows for an estimation of the thermal expansion coefficient during isothermal processes. Caloric and optical studies show a differing behavior as a function of the nanoparticle concentration that will be in the focus of the discussion.

CPP 49.3 Fri 10:45 H48

Theory of light-induced deformation of azobenzene elastomers — •Vladimir Toshchevikov[1,2], Marina Saphiannikova[1], and Gert Heinrich[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden, Germany — [2]Institute of Macromolecular Compounds, Bolshoi pr. 31, 199004 Saint-Petersburg, Russia

Photosensitive elastomers bearing azobenzene moieties in their strands are able to change the shape under light irradiation. These polymers have a fascinating potential for technical applications as smart materials (microrobots, micropumps, artificial muscles). Recently, we have proposed a microscopic theory [1] of light-induced deformations in amorphous azobenzene polymers consisting of short oligomers which bear azobenzene moieties in their side chains. In the present work we extend the theory [1] to azobenzene elastomers taking the chain structure of network strands explicitly into account. We show that similar to the amorphous azobenzene polymers the photo-elastic behaviour of azobenzene elastomers is very sensitive to their chemical structure. Depending on it, a sample can be either stretched or uniaxially compressed along the electric vector of the linearly polarized light. For some chemical structures, elongation of a sample displays a nonmonotonic behaviour with the light intensity. The results of the theory are compared with experimental data for azobenzene elastomers.

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

[1] V.Toshchevikov, M.Saphiannikova, G.Heinrich. J. Phys. Chem. B 2009, 113, 5032.

CPP 49.4 Fri 11:00 H48

Magnetically induced surface instabilities in a thermoreversible ferrogel — •Tobias Lang[1], Christian Gollwitzer[1], Marina Krekhova[2], Günther Lattermann[2], Ingo Rehberg[1], and Reinhard Richter[1] — [1]Experimentalphysik V, Universität Bayreuth — [2]Makromolekulare Chemie I, Universität Bayreuth

The viscoelastic properties of thermoreversible ferrogels [1] can be tuned via temperature variation, making them an exciting type of magnetic soft matters. We study the formation of surface instabilities in a layer of thermoreversible ferrogel when exposed to a homogenous vertical magnetic field. The dynamics of the surface evolution is recorded using an specialized X-ray technique [2]. The ferrogel samples are characterized using rheological and magnetometer measurements. The critical magnetic field for the formation of Rosensweig cusps [3] is determined and compared to theoretical predictions [4]. In a conduction to [5] the growth rates of the emerging Rosensweig patterns are measured.

[1] G. Lattermann and M. Krekhova, Macromol. Rapid. Commun. 27, 1273 (2006)

[2] R. Richter and J. Bläsing, Rev. Sci. Instrum. 72, 1729 (2001)

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

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

[5] C. Gollwitzer, M. Krekhova, G. Lattermann, I. Rehberg, R. Richter, Soft Matter 5, 2093 (2009)

CPP 49.5 Fri 11:15 H48

Segmental order of entangled polymer networks is controlled by monomer fluctuations along the confining tube — •Michael Lang and Jens-Uwe Sommer — Leibniz Institut für Polymerforschung, Hohe Straße 6, 01069 Dresden

The tube model of entangled chains is applied to compute segment fluctuations and segmental orientational order parameter in polymer networks. The latter is essential for interpreting NMR measurements of entangled polymer networks. The sliding motion of monomers along the tube axis leads to a non-homogeneous reduction of segmental order along the chain. For network strands of length N much larger than entanglement length N_e, the average segmental order decreases $\sim (N_eN)^{-1/2}$ in marked contrast to the $1/N_e$ contribution of entanglements to network elasticity. As consequence, network modulus is not proportional to segmental order in entangled polymer networks. Monte Carlo simulation results of polymer networks over a wide range of molecular weights are in quantitative agreement with the theoretical predictions. The impact of entanglements on these properties is directly tested by comparing with simulations where entanglement constraints are switched off.

CPP 49.6 Fri 11:30 H48

NMR observation of "quantized" defect structures in hydrogels — •Frank Lange[1], Takamasa Sakai[2], and Kay Saalwächter[1] — [1]Institut für Physik - NMR , Betty-Heimann-Str. 7, 06120 Halle, Germany — [2]Department of Bioengineering, School of Engineering, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

We present data on a new class of hydrogels, the so called Tetra-PEG. These biodegradable gels are made from four-arm macromers with well-defined molecular weight. End-linking of the precursor macromers in semi-dilute solution results in gels with a highly homogeneous microstructure and advanced mechanical properties, in contrast to conventional hydrogels, which are usually very heterogeneous. Investigations were performed at a low-field NMR spectrometer with a proton multiple-quantum pulse sequence.

Analysis of the data shows a step-like increase of the normalized double-quantum buildup curve, which is due to a well-defined microscopic defect structure of the hydrogels. Such unique structural details are here observed for the first time. The observation becomes possible because of the unique overall homogeneity of the samples. The residual dipolar coupling constant derived from the buildup curves is proportional to the inverse of the network chain molecular weight, and based on this we conclude that the defects are due to multi-linking between two macromers. The dependence of the amounts and types of defects on various parameters such as concentration or stoichiometry variations is investigated in detail.

CPP 49.7 Fri 11:45 H48

Coupling strength between optical polarizability and structural formation during the chemically induced gelation and glass transition in epoxies — •Martine Philipp[1], Carsten Wehlack[2], Wulff Possart[2], Ulrich Müller[1], Roland Sanctuary[1], and Jan Krüger[1] — [1]Laboratory for condensed matter physics, University of Luxembourg, Luxembourg — [2]Lehrstuhl für Adhesion und Interphasen in Polymeren, Universität des Saarlandes, Germany

The chemically induced gelation and glass transition are investigated during the network formation in epoxies. The refractive index turns out to be astonishingly sensitive to structural formation close to the macroscopically isostructural phase transitions. Indeed, the evolution of the refractive index is not only determined by the mass density's behaviour, in the sense of the Lorentz-Lorenz relationship, but additional relevant contributions of the electronic polarizability at optical frequencies are evidenced. The gelation and the glass transition seem to influence the optical polarizability in strongly different manners. Topological disturbances, like nanoparticles will be shown to diminish the optical polarizability during gelation close to the sol-gel transition. High performance refractometry and infrared spectroscopy are combined as experimental techniques.

CPP 49.8 Fri 12:00 H48

Surface-near structuring of pressure sensitive adhesive films — •Alexander Diethert[1], Volker Körstgens[1], David Magerl[1], Yana Peykova[2], Olga Lebedeva[2], Norbert Willenbacher[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department LS E13, James-Franck-Str. 1, 85747 Garching (Germany) — [2]Universität Karlsruhe (TH), Institut für Mechanische Verfahrenstechnik und Mechanik, Gotthard-Franz-Str. 3, 76131 Karlsruhe (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. In the presented work we focus on the PSA model system P(EHA-stat-MMA) consisting of the tacky monomer ethyl hexylacrylate and the glassy monomer methyl methacrylate. The PSA films were prepared with solution casting.

In a previous x-ray reflectivity investigation we could prove the existence of enrichment layers of one type of monomer near the sample surface. Grazing incidence small angle x-ray scattering (GISAXS) experiments now added a new aspect: in addition to the layering also lateral structures are present. The data are modeled with cylindrical PMMA objects in a PEHA matrix. In particular, the evolution of the radii and the center-to-center distance during aging of the PSA film is quantified. Furthermore, the effect of this reorganization process on the adhesive properties is monitored with mechanical tack tests.