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

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Overview of Invited Talks and Sessions

(lecture rooms C 130, C 243, C 264, ER 270; Poster A)

Plenary, Keynote and Prize Talks related to Division CPP

PV III	Mon	14:00–14:45	ER 270	**Soft Matter and Life Sciences: Research with Neutrons** — •Dieter Richter
PV IV	Mon	14:00–14:45	HE 101	**Elementary excitations in single molecules on surfaces** — •Katharina J. Franke
PV IX	Tue	14:00–14:45	HE 101	**STM of Defects, Adsorbates, and Nanostructures at Oxide Surfaces** — •Ulrike Diebold
PV X	Tue	14:00–14:45	H 0104	**Terahertz Science and Technology: Key Innovations and Driving Applications** — •Karsten Buse
PV XI	Tue	17:20–18:00	H 0105	**Metamaterials and Transformation Optics** — •Martin Wegener
PV XIX	Thu	13:15–14:00	H 0105	**Mechanics and Growth of Tissues** — •Jean-Francois Joanny
PV XX	Thu	14:00–14:45	H 0105	**How superficial is adhesion? Common fundamentals of gecko, bacteria, protein and thin film adhesion** — •Karin Jacobs
PV XXIV	Fri	8:30– 9:15	H 0105	**Role of van der Waals Interactions in Physics, Chemistry, and Biology** — •Matthias Scheffler

Invited and Topical Talks

CPP 1.1	Mon	9:30–10:00	C 130	**Local anodic oxidation nanolithography on alkyl-terminated silicon surfaces: Chemical routes towards functional nanostructures** — •Harald Graaf, Maik Vieluf, Thomas Baumgärtel
CPP 2.8	Mon	11:30–12:00	C 243	**Gold nanoparticle assisted thermophoretic trapping of single nano-objects** — Marco Braun, Romy Schachoff, •Frank Cichos
CPP 3.1	Mon	9:30–10:00	ER 270	**Neither crystalline nor amorphous: how charge transport is affected by order in organic semiconductors** — •Alberto Salleo
CPP 3.7	Mon	11:45–12:15	ER 270	**Charge transport and recombination in organic light-emitting diodes** — •Paul Blom
CPP 4.1	Mon	15:00–15:30	C 243	**Glass transition by molecular network topology freezing and discovery of vitrimers** — •Ludwik Leibler, Damien Montarnal, Mathieu Capelot, François Tournilhac
CPP 4.2	Mon	15:30–16:00	C 243	**Elastic Properties of 2D amorphous solids** — •Peter Keim
CPP 5.1	Mon	15:00–15:30	ER 270	**Single-Molecule Spectroscopy of Conjugated Polymers: Unravelling Chain Conformations from the Bottom Up** — •John Lupton
CPP 5.5	Mon	16:15–16:45	ER 270	**Band dispersion and localized states in organic solids** — Nobuo Ueno, •Norbert Koch
CPP 10.1	Tue	9:30–10:00	C 130	**PEG Functionalized Lipid Bilayers at the Solid / Liquid Interface: Protrusions versus Blisters** — •Beate Klösgen, Giovanna Fragneto, Avi Halperin, Ole G. Mouritsen, Patricia Hardas, Michele Sferrazza
CPP 11.1	Tue	9:30–10:00	C 243	**Employing natural search strategies for complex optimization problems** — Christoph Schiffmann, •Daniel Sebastiani

CPP 28.1	Wed	15:00–15:30	C 130	**The glass transition is continuous but gelation is discontinuous in sticky spheres** — •Paddy Royall, Stephen Williams, Hajime Tanaka
CPP 29.1	Wed	15:00–15:30	C 243	**Observation of kinks and antikinks in colloidal monolayers driven across ordered surfaces** — •Thomas Bohlein, Jules Mikhael, Clemens Bechinger
CPP 29.2	Wed	15:30–16:00	C 243	**2D and 3D assembly of polymer-coated gold nanoparticles** — •Matthias Karg
CPP 30.1	Wed	15:00–15:30	C 264	**Soft Matter Research at the ESS** — •Ken Andersen
CPP 30.7	Wed	17:00–17:30	C 264	**Scanning small-angle X-ray scattering: Imaging nano-scale properties of extended samples** — •Oliver Bunk
CPP 31.1	Thu	9:30–10:00	C 130	**Large area flexible and stretchable electronics** — •Siegfried Bauer
CPP 32.1	Thu	9:30–10:00	C 243	**Stress relaxation and chain dynamics in entangled polymer melts** — •Ralf Everaers
CPP 32.5	Thu	10:45–11:15	C 243	**Slow stress relaxation in recoiling polymers** — •Ulrich F. Keyser
CPP 32.9	Thu	12:00–12:30	C 243	**Cytoskeletal stress in collective cell migration** — •Xavier Trepat
CPP 33.1	Thu	9:30–10:00	C 264	**Neutron Scattering Studies on Self-Healing Model Polymers** — •Ana Rita Brás, Jessalyn Cortese, Corinne Soulié-Ziakovic, François Tournilhac, Jürgen Allgaier, Wim Pyckhout-Hintzen, Andreas Wischnewski, Ludwik Leibler, Dieter Richter
CPP 33.6	Thu	11:15–11:45	C 264	**Shear inversion of polymer-brush bilayers with embedded colloids** — •Torsten Kreer, Andre Galuschko
CPP 34.1	Thu	15:00–15:30	C 130	**Colloidal quasicrystals: from their discovery to photonic applications** — •Stephan Förster, Alexander Exner, Sabine Rosenfeldt, Jan Perlich, Peter Lindner
CPP 35.1	Thu	15:00–15:30	C 243	**Motion of microswimmers governed by light in a fluid flow.** — •Philippe Peyla, Salima Rafaï, Xabel Garcia
CPP 36.1	Thu	15:00–15:30	C 264	**From superhydrophobic to superamphiphobic coatings: How to tune wetting** — •Doris Vollmer, Xu Deng, Lena Mammen, Periklis Papadopoulos, Hans-Jürgen Butt
CPP 38.1	Fri	9:30–10:00	C 130	**The Rheology of Biological Cells** — Mathias Sander, Benjamin Tränkle, Pablo Fernandez, Pramod Pullarkat, Lutz Heymann, Nuri Aksel, •Albrecht Ott
CPP 39.4	Fri	10:15–10:45	C 243	**Guided and spatio-selective transport via anisotropic fluid flows** — •Anupam Sengupta, Christian Bahr

Invited talks of the joint symposium SYXD

See SYXD for the full program of the symposium.

SYXD 1.1	Mon	15:00–15:30	H 0105	**Disputed discovery: The beginnings of X-ray diffraction in crystals** — •Michael Eckert
SYXD 1.2	Mon	15:30–16:00	H 0105	**Why are quasicrystals quasiperiodic?** — •Walter Steurer
SYXD 1.3	Mon	16:00–16:30	H 0105	**Coherent Diffraction Imaging with Free-Eletron Lasers** — •Massimo Altarelli
SYXD 1.4	Mon	16:30–17:00	H 0105	**X-ray free-electron lasers - emerging opportunities for structural biology** — •Ilme Schlichting
SYXD 1.5	Mon	17:00–17:30	H 0105	**Structure analysis by x-ray diffraction and x-ray imaging: beyond crystals, beyond averages, and beyond modeling** — •Tim Salditt

Invited talks of the joint symposium SYOL

See SYOL for the full program of the symposium.

SYOL 1.1	Fri	9:30–10:00	H 0105	**From sequence to function: Random polymerization and modular evolution of RNA** — •Susanna C. Manrubia
SYOL 1.2	Fri	10:00–10:30	H 0105	**Spontaneous autocatalysis and periodic switching in a prebiotic broth** — •Eva Wollrab, Sabrina Scherer, Karsten Kruse, Albrecht Ott
SYOL 1.3	Fri	10:30–11:00	H 0105	**Thermal solutions for molecular evolution** — •Dieter Braun
SYOL 1.4	Fri	11:00–11:30	H 0105	**Systems chemistry: Self-replication and chiral symmetry breaking** — •Guenter von Kiedrowski

Sessions

CPP 1.1–1.13	Mon	9:30–13:15	C 130	**Interfaces and Thin Films I**
CPP 2.1–2.13	Mon	9:30–13:15	C 243	**Nanoparticles and Composite Materials**
CPP 3.1–3.11	Mon	9:30–13:15	ER 270	**Focus: Structural Ordering and Electronic Transport I (joint focus with HL)**
CPP 4.1–4.8	Mon	15:00–17:30	C 243	**Glasses I (joint session with DY)**
CPP 5.1–5.8	Mon	15:00–17:30	ER 270	**Focus: Structural Ordering and Electronic Transport II (joint focus with HL)**
CPP 6.1–6.29	Mon	17:30–19:30	Poster A	**Poster: Structural Ordering and Electronic Transport (joint focus with HL)**
CPP 7.1–7.10	Mon	17:30–19:30	Poster A	**Poster: Biopolymers and Biomaterials (jointly with BP)**
CPP 8.1–8.50	Mon	17:30–20:00	Poster A	**Poster: Nanoparticles and Composite Materials**
CPP 9.1–9.12	Tue	9:30–13:00	H 1058	**Biopolymers and Biomaterials (joint session with BP)**
CPP 10.1–10.12	Tue	9:30–13:00	C 130	**Interfaces and Thin Films II**
CPP 11.1–11.12	Tue	9:30–13:00	C 243	**New Instruments and Methods**
CPP 12.1–12.10	Tue	10:00–12:30	MA 004	**Glasses II (joint session with DY)**
CPP 13.1–13.36	Tue	18:15–20:45	Poster A	**Poster: Interfaces and Thin Films**
CPP 14.1–14.17	Tue	18:15–20:15	Poster A	**Poster: Glasses I (jointly with DY)**
CPP 15.1–15.19	Tue	18:15–20:15	Poster A	**Poster: New Instruments and Methods**
CPP 16.1–16.46	Tue	18:15–20:45	Poster A	**Poster: Colloids and Complex Liquids**
CPP 17.1–17.21	Tue	18:15–20:15	Poster A	**Poster: Crystallisation, Nucleation and Self assembly**
CPP 18.1–18.6	Wed	9:30–11:00	C 130	**Organic semiconductors I**
CPP 19.1–19.6	Wed	9:30–11:00	C 243	**Charged Soft Matter**
CPP 20.1–20.6	Wed	9:30–11:00	C 264	**(Hydro)gels and Elastomers**
CPP 21.1–21.23	Wed	11:00–13:00	Poster A	**Poster: Wetting, Micro and nanofluidics**
CPP 22.1–22.18	Wed	11:00–13:00	Poster A	**Poster: Charged Soft Matter**
CPP 23.1–23.15	Wed	11:00–13:00	Poster A	**Poster: Polymer Dynamics**
CPP 24.1–24.33	Wed	11:00–13:00	Poster A	**Poster: Organic Semiconductors**
CPP 25.1–25.11	Wed	11:00–13:00	Poster A	**Poster: Stress Relaxation in Polymers - From single molecules to biological cells (joint focus with BP)**
CPP 26.1–26.8	Wed	11:00–13:00	Poster A	**Poster: New Perspectives of Scattering at Soft Matter**
CPP 27.1–27.17	Wed	11:00–13:00	Poster A	**Poster: (Hydrogels) and Elastomers**
CPP 28.1–28.13	Wed	15:00–18:45	C 130	**Colloids and Complex Liquids I**
CPP 29.1–29.12	Wed	15:00–18:45	C 243	**Crystallisation, Nucleation and Self assembly**
CPP 30.1–30.12	Wed	15:00–18:45	C 264	**New Perspectives of Scattering at Soft Matter**
CPP 31.1–31.11	Thu	9:30–12:45	C 130	**Organic semiconductors II**
CPP 32.1–32.9	Thu	9:30–12:30	C 243	**Focus: Stress Relaxation in Polymers - From single molecules to biological cells (joint focus with BP)**
CPP 33.1–33.9	Thu	9:30–12:30	C 264	**Polymer Dynamics**
CPP 34.1–34.13	Thu	15:00–18:45	C 130	**Colloids and Complex Liquids II**
CPP 35.1–35.13	Thu	15:00–18:45	C 243	**Focus: Rheology I (joint focus with DRG)**
CPP 36.1–36.13	Thu	15:00–18:45	C 264	**Wetting, Micro and nanofluidics I**
CPP 37.1–37.10	Thu	18:45–19:45	Poster A	**Poster: Rheology (joint focus with DRG)**
CPP 38.1–38.10	Fri	9:30–12:15	C 130	**Focus: Rheology II (joint focus with DRG)**
CPP 39.1–39.9	Fri	9:30–12:00	C 243	**Wetting, Micro and nanofluidics II**

Annual General Meeting of the Chemical and Polymer Physics Division

Wednesday 19:00–20:00 C130

- Report
- Election Vice-Spokeperson
- Conference 2013
- CPP Poster prize
- Other topics

CPP 1: Interfaces and Thin Films I

Time: Monday 9:30–13:15 Location: C 130

Topical Talk CPP 1.1 Mon 9:30 C 130

Local anodic oxidation nanolithography on alkyl-terminated silicon surfaces: Chemical routes towards functional nanostructures — •Harald Graaf[1,2], Maik Vieluf[1], and Thomas Baumgärtel[1] — [1]Chemnitz University of Technology, Institute of Physics, Germany — [2]Kassel University, Institute of Chemistry, Germany

The structuring of surfaces on a nanometer scale is one of the demands that have to be fulfilled in order to advance the design and to aspire to miniaturisation in semiconductor technologies. Besides further development of conventional optical lithography, alternative lithography techniques are in the focus of recent research to achieve lateral structures on the nanometer scale. Here scanning probe based lithography (SPL) is one of the emerging fields. One SPL approach is the local anodic oxidation (LAO) where a voltage is applied between scanning probe microscopy (SPM) tip and sample surface leading to an electrochemical oxidation reaction. In the case of an (alkyl-terminated) silicon sample, the silicon is oxidized locally at the tip apex forming silicon oxide structures. The chemically different oxide can afterwards be altered through the attachment of molecules or nanoparticles in order to give the structures a defined functionality. In this talk, basics of the LAO technique will be introduced and an overview will be given of the research in that field both regarding the understanding of the process itself as well as possible applications to generate functionalized structures. This contribution will thereby deal on the optical properties of prepared functional nanostructures.

CPP 1.2 Mon 10:00 C 130

Low temperature route to nano-structured crystalline titania thin films — •Monika Rawolle[1], Christian Gebbe[1], Erik V. Braden[1], Martin A. Niedermeier[1], David Magerl[1], Kuhu Sarkar[1], Volker Körstgens[1], Thomas Fröschl[2], Nicola Hüsing[2], Jan Perlich[3], Adeline Buffet[3], Stephan V. Roth[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]Universität Salzburg, Materialforschung und Physik, 5020 Salzburg, Austria — [3]HASYLAB at DESY, 22603 Hamburg, Germany

A low temperature route to crystalline titania thin films is presented, which is interesting for inorganic-organic hybrid photovoltaics due to lower costs, easy producibility and the possibility of using organic flexible substrates. An ethylene glycol modified titanate (EGMT) precursor yields crystalline titania already at low temperatures, where the crystal phase (anatase or rutile) depends on the pH value.[1] We use this precursor to prepare thin films with well-defined nanostructures. The nano-structure is controlled with a diblock copolymer as templating agent combined with sol-gel chemistry. The nano-morphology is investigated with SEM, XRR and GISAXS. Crystallinity is determined with GIWAXS and related to optical properties as probed with UV/Vis spectroscopy. Solar cells prepared with titania derived from EGMT are characterized electronically under illumination with a solar spectrum (AM 1.5).

[1] Denkwitz et al., J. Appl. Catal. B:Environ. (2009) 91, 470.

CPP 1.3 Mon 10:15 C 130

Imaging of carbon nanomembranes with helium-ion microscopy — •Andre Beyer, Andrey Turchanin, and Armin Gölzhäuser — Physics of Supramolecular Systems, University of Bielefeld, 33615 Bielefeld, Germany

Helium-ion microscopy (HIM) is similar to scanning electron microscopy but it employs helium ions for scanning a sample instead of electrons. The resulting images are more surface sensitive with a higher resolution as compared to scanning electron microscopy. Here we present a study about imaging extremely thin nano-scale objects: carbon nanomembranes which consist exclusively of atoms near the surface. Such freestanding nanomembranes with a thickness of 1 nm are made from self-assembled monolayers (SAMs) by cross-linking and subsequent transfer to transmission electron microscopy (TEM) grids or other suitable substrates. We show that these nanomembranes exhibit a substantially higher contrast in helium-ion microscopes as compared to electron microscopes. Cross-linking of SAMs is performed by large area exposures with electrons or photons which yield extended nanomembranes. On the other hand, patterned exposures allow the fabrication of nanosieves, i.e. perforated nanomembranes. Advantages in imaging such patterned cross-linked SAMs as well as freestanding nanosieves with the helium-ion microscope will be discussed.

CPP 1.4 Mon 10:30 C 130

Improvement of Adsorption Stability of Indoline Sensitizers in Dye-Sensitized Solar Cells by Additional Binding Groups — •Jane Falgenhauer[1], Hidetoshi Miura[2], and Derck Schlettwein[1] — [1]Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen — [2]Tsukuba Research Center, Chemicrea Inc., D-142-1-6, Sengen, Tsukuba, Ibaraki 305-0047, Japan

Dye-sensitized solar cells often suffer from desorption of sensitizer molecules during operation and in contact to a redox electrolyte. In particular for ZnO as active semiconductor material, an optimal dye has still to be found. In this study, novel indoline dyes with additional binding groups to the semiconductor surface were investigated. Their adsorption stability on ZnO was studied in comparison with the established indoline dye $D149$. The dyes were adsorbed on nanoporous electrodeposited ZnO with a co-adsorbent, chenodeoxycholic acid. The amount of dyes adsorbed to the films was measured by optical absorption spectroscopy. Under operation in contact to a typical redox electrolyte, the dyes showed different desorption probability. The amount of desorbed dyes in such a solution containing the electrolyte additive $N - Methylbenzimidazole(NMBI)$ was also investigated by optical absorption spectroscopy, as well as the absorption of the films following these desorption experiments. The stability of the dyes in dependence on the number of binding groups at the sensitizer molecules will be discussed.

CPP 1.5 Mon 10:45 C 130

Stretchable metal films on ultrathin substrates — •Michael Drack, Martin Kaltenbrunner, Ingrid Graz, and Siegfried Bauer — Soft Matter Physics, Institute Experimental Physics, J. Kepler University, Altenbergerstraße 69, 4040 Linz, Austria

Today's electronic devices are rigid, tomorrow's electronics is expected to be used everywhere. Conformability will be the key to use electronics everywhere: electronic textiles, ultra-conformable solar panels and stretchable sensor skins are just a few potential applications. Unfortunately most electronic materials are brittle and fracture at 1% strain. Metals are ductile but plastically deform and break. So the question arises how to make such brittle or plastically deformable materials mechanically stretchable.

Here we present an approach to make thin metal electrodes mechanically highly compliant. The metal electrodes are fabricated by thin film processing techniques onto an ultrathin and ultra-flexible polymer substrate. A 1.4 micron thick PEN polymer foil is used as the substrate for the metal films. On a pre-stretched and relaxed elastomer, the metal electrodes on the thin PEN substrate form wrinkles. We have found that such 100nm thick aluminium, copper, gold and silver electrodes can be reversibly stretched uniaxially to 50% for 1000 cycles without failure. Their electrical resistance does not change significantly with cycling, paving ways for making any metal film mechanically stretchable.

CPP 1.6 Mon 11:00 C 130

Light-induced wrinkling and moving gratings in low-molecular azo films — Philipp Gruner, Michael Arlt, and •Thomas Fuhrmann-Lieker — Makromolekulare Chemie und Molekulare Materialien, Universität Kassel

The dynamics of mass transport in thin layers of a low molecular glass containing azo chromophores are studied in two experiments.

First, spinodal wrinkling of a multilayer system consisting of the azo glass confined by a rigid substrate and an elastic cover layer is induced by light. The time evolution of the wrinkle structures is measured and compared to thermal wrinkling. Application of theoretical models allows the determination of the viscoelastic properties in the non-equilibrium fluid.

Second, in a dynamic holographic experiment surface corrugation gratings are shifted by phase control of the generating beams. The relaxation timescale in which the corrugation pattern can follow the moving light field is measured.

With these experiments, fundamental properties of photofluidic thin films such as irradiation-dependent viscosity are addressable.

15 min break

CPP 1.7 Mon 11:30 C 130

Self-assembled membranes from bionanoparticle-polymer conjugates — •Patrick van Rijn, Nathalie Mougin, Christine Kathrein, and Alexander Böker — DWI an der RWTH Aachen e.V., IPC RWTH Aachen University, Germany

New bionanoparticles have been prepared by using Horse spleen Ferritin (HSF) as a scaffold for the grafting from of thermo-responsive poly(N-isopropyl acrylamide) and photo-cross-linkable (2-(dimethyl maleinimido)-N-ethyl-acrylamide. The amino-groups on the exterior of HSF were modified to form a macro-initiator from which sequentially atom transfer radical polymerization was performed.[Mougin, et. al. Adv. Funct. Mater. 2011, 21, 2470] The newly formed bionanoparticles-polymer composites are excellent candidates for the stabilization of polar/apolar interfaces.[van Rijn, et. al., Langmuir, submitted] and oil-in-water and water-in-oil emulsions have been prepared and stabilized by cross-linking, forming soft capsules which are stable enough to be collected, transferred and are able to endure cosolvents like ethanol.[van Rijn, et. al. Chem. Commun., 2011, 47, 8376] A similar process can also be used for the formation of 2-D membranes which display interesting properties. Here the protein is used as a sacrificial template which creates defined pores after denaturation. The membranes are highly stable, easily formed and used for the separation of various nano-sized species.

CPP 1.8 Mon 11:45 C 130

Stimuli-responsive surfaces based on triblock terpolymer micelles — •Julia Gensel[1], Eva Betthausen[2], Inna Dewald[1], Johann Erath[1], Fouzia Boulmedais[3], Axel H. E. Müller[2], and Andreas Fery[1] — [1]Physical Chemistry II, University of Bayreuth, Germany — [2]Macromolecular Chemistry II, University of Bayreuth, Germany — [3]Institut Charles Sadron, Université de Strasbourg, France

The surface adsorption of stimuli-responsive block copolymer micelles on a solid substrate leads to stimuli-responsive coatings with well defined thickness and morphology. In this contribution we present a novel approach for the design of stimuli-responsive surfaces based on the deposition of charged pH-responsive core-shell-corona micelles.[1]

The adsorption of these micelles on silica is adequately described by the Random Sequential Adsorption model. By variation of the solution pH, it is possible to reversibly switch the surface micelles' charge density, swelling state and composition.[2] These switchable surfaces can be used as active surfaces for bio-applications for example for the controlled self-regulated bacteria release.

Using the layer-by-layer approach, the micelles are included within multilayer films with tailored nanostructure and integrated pH-responsive properties. The film swelling degree, morphology as well as the mechanical properties of the coatings are tunable by the solution pH. These systems are potentially interesting as nano-actuators.

[1] E. Betthausen et al., Soft Matter, 2011, 7, 8880-8891.

[2] J. Gensel et al., Soft Matter, 2011, 11144-11153.

CPP 1.9 Mon 12:00 C 130

Guiding block copolymers into sequenced patterns via inverted terrace formation — •Sungjune Park[1], Larisa Tsarkova[1], Stephanie Hiltl[1], Stefan Roitsch[2], Joachim Mayer[2], and Alexander Böker[1] — [1]DWI an der RWTH Aachen e. V., Lehrstuhl für Makromolekulare Materialien und Oberflächen, RWTH Aachen University, D-52056 Aachen, Germany. — [2]Gemeinschaftslabor für Elektronenmikroskopie, RWTH Aachen University, Ahornstr. 55, D-52074 Aachen, Germany.

We present a facile one-step route to achieve sequenced patterns from microphase separated structures in asymmetric polystyrene-b-polybutadiene (PS-b-PB) diblock copolymer films. For the guided block copolymer assembly we used topographically corrugated SiCN ceramic substrates which were fabricated by a facile replication process using non-lithographic PDMS masters. Homogeneous block copolymer films have been floated onto the corrugated substrate without significant changes to the corrugations topography. During thermal annealing of PS-b-PB diblock copolymer, the material transport was guided by a wrinkled substrate to form regular modulations in the film thickness. As a consequence of the thickness-dependent morphological behavior, the film surface appears as sequenced patterns of alternative microphase separated structures. The ordering process is attributed to a newly observed phenomenon of inverted terrace formation which is induced by the corrugations on substrate, so that the resulting surface patterns are free from the surface relief structures within macroscopically large areas.

CPP 1.10 Mon 12:15 C 130

Influence of interface interactions on the inner structure of pressure sensitive adhesive films — •Markus Schindler[1], Armin Kriele[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany — [2]TU München, Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Lichtenbergstr.1, 85748 Garching, Germany

Pressure sensitive adhesives (PSAs) are widely used in everyday applications, industries and medicine, although surprisingly still lacking fundamental understanding on molecular scale. Individually tailored compounds exist for almost every possible environment, in which they still allow for reversible adhesion. Previous studies on our model system consisting of the statistical copolymer poly(ethylhexylacrylate-stat-methylmethacrylate) have shown that the two components of the polymer establish enrichment layers at the top surface that significantly affect the tack performance. We present insights into the internal reorganization of the solution cast adhesive films' inner structure upon different interface interactions which makes it possible to apply the same adhesive for higher and lower tack applications. The timescale on which these changes of the inner structure take place also provides information about the durability of established adhesive bonds. We present a study on the influence of an unpolar nitrogen atmosphere on the internal reorganization with time of adhesive films showing a complete inversion of the layering installed during the sample preparation.

CPP 1.11 Mon 12:30 C 130

Decelerating dewetting by shining light on a thin polymer film containing conjugated molecules — •Ioan Botiz[1,2], Natalie Stingelin[3], and Günter Reiter[1,2] — [1]Freiburg Research Institute for Advanced Studies — [2]Institute of Physics, University of Freiburg — [3]Imperial College London

We use an induced dewetting process as a method to control polymer conformations by stretching molecules within an ultrathin residual layer in the dewetting direction. Varying physical parameters like temperature, substrate type, light intensity, film thickness and age, we control the dewetting velocity, the final patterns (droplets and the residual thin layer), including the degree of molecular stretching. We show that, under nitrogen conditions, light intensity decelerates by two folds the dewetting velocity of a thin film of conjugated Poly[2-methoxy-5-((2'-ethylhexyl)oxy)-1,4-phenylenvinylene] (MEH-PPV) molecules embedded in an optically inert polystyrene matrix. No light effect is observed in thin films of polystyrene alone. Switching the light on and off leads to deceleration and acceleration of dewetting respectively, indicating a reversible effect of light. We attempt to explain our experimental observations suggesting that light induces new electronic states in MEH-PPV molecules (most probably long lived triplet states) leading to a change in molecular conformation characterized by a higher chain rigidity and therefore a higher polymer viscosity, i.e. lower dewetting velocity.

CPP 1.12 Mon 12:45 C 130

In-situ study of structural changes in lamellar diblock copolymer thin films during heat treatment — •Alessandro Sepe[1], Dorthe Posselt[2], Jan Perlich[3], Detlef-M. Smilgies[4], and Christine M. Papadakis[1] — [1]TU München, Physikdepartment, Physik weicher Materie, Garching, Germany — [2]Institute for Science, Systems and Models, Roskilde University, Denmark — [3]HASYLAB at DESY, Hamburg — [4]Cornell High-Energy Synchrotron Source (CHESS), Ithaca, U.S.A.

Diblock copolymer thin films are prominent candidates for a range of applications requiring nanostructured surfaces, such as nanoporous films. Thermal annealing has frequently been applied to remove defects and to improve the long-range order. Annealing temperature is a key parameter because it influences both, the interfacial tension between the two blocks and the polymer mobility. We investigate the mechanisms of structural changes induced by thermal treatment of thin films of poly(styrene-*b*-butadiene) having initially the perpendicular lamellar orientation. In-situ grazing-incidence small-angle X-ray scattering and VIS interferometry as well as ex-situ atomic force spectroscopy and X-ray reflectivity were used to monitor the changes. We have found that for annealing temperatures below the glass transition temperature of the PS block and subsequent cooling to room temperature, the lateral order is improved, whereas above, a random lamellar orientation and subsequent severe changes of the film structure are observed.

CPP 1.13 Mon 13:00 C 130

Stability and Orientations of Lamellae in Confined Block Copolymer Films — •Vanessa Weith, Alexei Krekhov, and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany

The study of self-assembly of block copolymers offers substantial opportunities to control the morphology of the evolving patterns. This is of considerable fundamental and technological importance for developing new materials to achieve specific properties.

Microphase separation in block copolymers is described by a two-dimensional mean-field model and its stationary, spatially periodic solutions are investigated for unconfined systems and for systems confined between two parallel boundaries having either equal or different wetting properties.

We determine the different stability and existence ranges of the periodic solutions in one and two spatial dimensions as well as the effects of confinement and of the block copolymer surface interaction on the free energy of lamellar solutions. This helps to determine which orientation of the lamellae is selected depending on the input parameters.

Furthermore the spatio-temporal behavior of the phase separation process of confined block copolymers is characterized.

CPP 2: Nanoparticles and Composite Materials

Time: Monday 9:30–13:15 Location: C 243

CPP 2.1 Mon 9:30 C 243

Fabrication of metamaterials by colloidal mask templating and glancing angle deposition: An in situ grazing incidence X-ray scattering study — •Jan Perlich[1], Adeline Buffet[1], Matthias Schwartzkopf[1], Mottakin M. Abul Kashem[1], Gerd Herzog[1], Kai Schlage[1], Ezzeldin Metwalli[2], Volker Körstgens[2], Ralf Röhlsberger[1], Peter Müller-Buschbaum[2], Stephan V. Roth[1], and Rainer Gehrke[1] — [1]HASYLAB-DESY, Hamburg (Germany) — [2]TU München, Physik Department, LS Funkt. Mat., Garching (Germany)

Metamaterials are artificially structured materials which attain their properties from the unit structure rather than the constituent materials using small inhomogeneities. Metamaterials have become a new subdiscipline in physics and their widespread areas of application include optics and optoelectronics, electromagnetics, microwave and antenna engineering, semiconductors, etc. We present the fabrication of such a metamaterial by sputter deposition of gold on colloidal polystyrene nanoparticles acting as shadowing mask. The gold is deposited under a glancing angle (GLAD) resulting in asymmetrically shaped gold-capped polystyrene nanospheres. The sputtering process is monitored in situ real-time by grazing incidence small angle X-ray scattering (GISAXS) performed at the synchrotron beamline P03 of PETRA III enabling millisecond time resolution. The characterization is complemented by scanning electron microscopy, yielding high-resolution images of the final morphology, and ellipsometry to determine the optical properties of the nanostructured material.

CPP 2.2 Mon 9:45 C 243

Molecular dynamics study of tracer diffusion in hairy nanochannel: normal vs anomalous — •Rajarshi Chakrabarti, Stefan Kesselheim, Peter Košovan, and Christian Holm — Institute for Computational Physics, Universität Stuttgart, Pfaffenwaldring 27, 70569, Stuttgart, Germany

We carry out extensive molecular dynamics simulation to analyze the diffusion of tracer particles inside a cylindrical nano-channel randomly grafted inside with polymeric chains. We show that depending on the attraction between the tracer and the polymer an intermediate subdiffusive behavior along the cylindrical axis can be observed but the long time diffusion is always normal. We also analyze the dependence of diffusion coefficient on the volume fraction of the grafted polymeric chains. Although simple the model presented here has the features of nuclear pore complex in the context of biological transport.

CPP 2.3 Mon 10:00 C 243

Diblock Copolymer - Selective Nanoparticle Mixture in Lamellar Phase Confined between two Parallel Walls : A Mean Field Model — •Lenin Singh Shagolsem[1,2] and Jens-Uwe Sommer[1,2] — [1]Leibniz Institute of Polymer Research Dresden, Dresden, Germany — [2]Institute of Theoretical Physics, TU Dresden, Dresden, Germany

We present a mean field model for a mixture of AB diblock-copolymers and A-block selective nanoparticles confined between two identical non-selective walls. A horizontally symmetric lamellar structure of the nanocomposite is considered. For a given nanoparticle volume fraction, ϕ, and wall separation, L, we study the change in the free energy as a function of the number of lamellar layers, p, and the nanoparticle uptake of the polymer film, $y = \phi x$, where $0 \leq x \leq 1$. We observe that there exists a particular p which is commensurable with the given film thickness. At small values of y, the equilibrium-uptake is mainly controlled by the balance of stretching, and the interaction between monomers and nanoparticles . We find that the equilibrium value of y is independent of ϕ and increase sub-linearly with monomer-nanoparticle interaction strength. In addition, we also consider A-block selective walls. Here, we investigate the non-wetting/wetting transition and constructed a corresponding phase diagram.

CPP 2.4 Mon 10:15 C 243

Assembly of nanoparticles on diblock copolymer brushes: toward laterally nanostructured composites — •Olga Guskova[1] and Christian Seidel[2] — [1]Leibniz Institute of Polymer Research, Dresden, Germany — [2]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

We study the self-assembly of polymer-unsoluble nanoparticles (NPs) at the surface of microphase-separated AB diblock copolymer brushes in a selective solvent by means of dissipative particle dynamics (DPD) simulations. The structure of such nanocomposites depends both on the morphology of the underlying brush which is basically determined by chain composition f and solvent selectivity t(B), and on specific parameters of the NPs added such as polymer compatibility a(BP), solvophobicity a(PS), and concentration c, where a(ij) are the DPD interaction parameters. The immense parameter space is explored within a coarse grained model that contains polymer A and B beads, solvent (S), nanoparticle (P), and wall (W) beads. For composites with B-like nanoparticles, i.e., NPs that are covered by polymer B ligands, we construct the phase diagram in the f-c space. For B-unlike NPs, it is found that the solvophobicity of the particles set by a(PS) is crucial for the spreading of the nanodroplets. We show that in principle microphase separated diblock copolymer brushes can be used to create ordered nanodots as well as nanowires and deduce some rules which should facilitate the design of such novel polymer nanocomposites.

CPP 2.5 Mon 10:30 C 243

Assembly of nanoparticles on hard surfaces and surface-grafted polyelectrolyte brushes — •Züleyha Yenice and Regine von Klitzing — Technische Universität Berlin, Stranski-Laboratorium, Department of Chemistry, Strasse des 17. Juni 124 D-10623 Berlin, Germany

Self-assembly of nanoparticles using modified surfaces like polymer brushes, surface grafted molecular and macromolecular gradients attract great interest in recent years [1,2].

Here, we present our studies on self-assembly of nanoparticles on bare silicon wafer and wafers modified by PDMAEMA brushes. PDMAEMA is a weak polyelectrolyte with pH dependent properties which gives us space to do further modifications on this brushes. We also present our effort to get a better understanding of the particle interpenetration into the polyelectrolyte brushes by investigating the effect of different brush lengths and different sizes of nanoparticles using x-ray reflectivity, ellipsometry and atomic force microscopy.

[1] J. Genzer and R. R. Bhat, Langmuir, Vol. 24, No. 6, 2008

[2] R. R. Bhat et al. Nanotechnology, 14 (2003) 1145-1152

CPP 2.6 Mon 10:45 C 243

Block Copolymer - Nanoparticle Composites in Electric Fields — •Clemens Liedel, Kerstin Schindler, Christian Wilhelm Pester, and Alexander Böker — Lehrstuhl für Makromolekulare Materialien und Oberflächen, DWI an der RWTH Aachen e.V., RWTH Aachen University, D-52056 Aachen, Germany

The creation of thin and densely-packed metallic wires is of key importance for creating new devices for electronic applications. Because of its size, block copolymers and metal nanoparticles are promising materials for this purpose. By creating composite materials from both, it is possible to combine the possibility of orienting block copolymer structures in electric fields with the conductivity of metal nanoparticles. Hence, ordered metallic structures are accessible.

We present a deeper understanding of nanoparticle - block copolymer composites in electric fields. Therefore, we show the influence of nanoparticles on the field strength that is necessary for aligning the morphologies. In addition, we describe the impact on the kinetics of orientation and the resulting order parameter.

Understanding composites from block copolymers and nanoparticles in electric fields may help to build new devices in the field of optical gratings, data storage or organic-inorganic solar cells.

CPP 2.7 Mon 11:00 C 243

Reactive epoxies with functional zeolite fillers: IR spectroscopy and PALS studies — •Klaus Rätzke[1], Qasim Shaikh[1], Jan Gaukler[2], Wulff Possart[2], and Franz Faupel[1] — [1]Materials Science Univ. Kiel, Germany — [2]Adhesion and Interphases, Materials Science, Saarbrücken, Germany

Epoxy-dicyandiamide (Dicy) formulations frequently contain a free accelerator for reducing the curing temperature and the time for network formation. However, an accelerator reduces the shelf life of these adhesives. This study compared the reaction kinetics during the storage at 60 °C for a pre-cured epoxy adhesive (EP = diglycidyl ether of bisphenol A and Dicy, mass ratio 100 : 6.7, pre-cured at 150 °C for 1 h) mixed either with free accelerator or with the same concentration of accelerator immobilised in micro or nano-zeolite fillers [1]. During storage, the IR study probed the chemical modifications. They lead to increasing crosslinking density and a loss of free volume as detected by positron annihilation lifetime spectroscopy (PALS) [2]. Crosslinking proceeds to the chemical vitrification. Additionally, the glass transition and the free volume parameters were investigated for the three systems as a function of temperature by PALS after thermal curing.

[1] K. Rätzke, M. Q. Shaikh, F. Faupel, P. L. M. Noeske International Journal of Adhesion & Adhesives, 30 (2010) 105

[2] M. Q. Shaikh, K. Rätzke, J. Ch. Gaukler, W. Possart, F. Faupel, J. Mater. Res., 26, (2011) 2877

15 min break

Topical Talk CPP 2.8 Mon 11:30 C 243

Gold nanoparticle assisted thermophoretic trapping of single nano-objects — Marco Braun, Romy Schachoff, and •Frank Cichos — Molecular Nanophotonics Group, University of Leipzig, Linnéstraße 5, D - 04103 Leipzig

Optical tweezing is the most common technique for the trapping of individual particles in solution. It is based on the gradient force of focused electromagnetic radiation. Hence, a sufficient high polarizability contrast between the particle and the solution is required. While it is thus easy to trap single dielectric particles larger than $100\,\mu$m, a trapping of smaller objects such as single molecules by means of an optical tweezer is hardly possible. Molecular trapping can be achieved by a technique called Anti-Brownian Elektrokinetic trap (ABEL trap), which exploits the time-dependent electric field of four electrodes. Here, we present a new technique which replaces the electric field by local thermal fields generated by single Au nanoparticles. The so-called Thermophoretic trap exploits thermophoretic forces that act on a particle placed in a temperature gradient, which e.g. locally distorts the screening of the surface charges. Such forces are sufficient for the manipulation of small nanoparticles or proteins. In our approach, the thermal gradient around optically heated Au nanoparticles immobilized in an appropriate arrangement shall be use to trap single nanoobjects. The plasmonic heating of the separate Au nanoparticles hereby is achieved by a focused laser beam that is controlled by a suitable feedback loop. Numerical simulations as well as first experimental results will be presented.

CPP 2.9 Mon 12:00 C 243

Determination of the three-dimensional orientation of gold nanorods by in-situ measuring their elastic scattering and luminescence signal — •Frank Wackenhut[1], Antonio Virgilio Failla[2], Tina Züchner[1], and Alfred J. Meixner[1] — [1]Eberhard Karls University, Institute of Physical and Theoretical Chemistry, Tübingen, Germany — [2]University Medical Center Hamburg-Eppendorf, Hamburg, Germany

We will demonstrate that it is possible to determine the three-dimensional orientation of a single gold nanorod (GNR) by simultaneously measuring the elastic scattering and luminescence pattern. For excitation we used radially and azimuthally polarized doughnut shaped modes (RPDM/APDM). In this work we will extend the results shown in [1] to a not index matched sample geometry. We will demonstrate that the combined acquisition of four patterns (luminescence and scattering patterns excited either by a RPDM or an APDM) allows us to determine the three-dimensional orientation of individual GNRs with high precision covering the full angular spectrum. In general the luminescence pattern is mainly used to determine the GNR orientation, while the acquisition of the scattering pattern in reflection mode permits us to gain additional information about the nano environment surrounding the GNR. This extends the results shown by Züchner et al. [2] to a 3D experimental system.

[1] F. Wackenhut, A.V. Failla, T. Züchner, A. J. Meixner, (2011). Proc. SPIE 8096 (1), 80962V. [2] T. Züchner, A. V. Failla, M. Steiner, A. J. Meixner, (2008). Opt. Express, 16; 14635-14644.

CPP 2.10 Mon 12:15 C 243

Cross-over in the power law statistics of the fluorescence of CdSe/CdS/ZnS nanocrystals — •Gerald Hinze and Thomas Basché — Institut für Physikalische Chemie, Johannes Gutenberg-Universität, 55099 Mainz

Semiconducting quantum dots (QD) are often characterized by bright luminescence and high photo stability compared to usual aromatic molecular dyes. On a single particle level, however, their fluorescence typically shows intermittencies. That is, under continuous light illumination stochastic jumps between light (on) and dark states (off) occur. At the same time the fluorescence decay from single QDs often cannot described by a single exponential. Recently, there have been attempts to explain both observations within a single model implementing an additional dark state. We have studied CdSe/CdS/ZnS colloidal quantum dot emission over 9 decades in time. By combining different experimental setups we were able to follow the temporal evolution of the fluorescence intensity of a bulk sample from ns to seconds. We observe three inverse power-laws differing in the exponent with cross over times at $\sim 100\mu$s and $\sim$5ms. From single molecule intensity time traces we calculated the off-time statistics related to the intermittency of the fluorescence. Within the accessible range of the off-time statistics, which was obtained for 3 decades of time, it nicely matches the time-dependent fluorescence intensity. Our results support the recent proposed model of diffusion-controlled electron transfer being the origin for the observed power law statistics.

CPP 2.11 Mon 12:30 C 243

Synthesis und characterization of selective sensor nanoparticles for magnetic resonance imaging — •Daniel Nordmeyer[1], Patrick Stumpf[1], Dominic Gröger[2], Florian Paulus[2], Rainer Haag[2], Annetta Semisch[3], Constanze Richter[3], Andrea Hartwig[3], Jens Dernedde[4], Ronny Malz[5], Ursula Rauch-Kröhnert[5], Jörg Schnorr[6], Ines Gemeinhardt[6], Matthias Taupitz[6], Christina Graf[1], and Eckart Rühl[1] — [1]Physikalische Chemie, FU Berlin — [2]Organische Chemie, FU Berlin — [3]Institut für Angewandte Biowissenschaften, Karlsruhe Institut für Technologie — [4]Institut für Laboratoriumsmedizin, Klinische Chemie und Pathobiochemie, Charité — [5]Centrum für Herz-, Kreislauf- und Gefäßmedizin, Charité — [6]Institut für Radiologie, Charité

The aim of the present study is the synthesis of iron oxide nanoparticles (FeOx-NP) functionalized by hyperbranched sulfated polyglycerols (hPGS, a heparin analogue) on their surfaces. This leads to antiinflammatory and antimetastatic effects in organism. Stability measurements with hPGS coordinated FeOx-NP are performed in different biological media. Human colon cancer cells are incubated with these hydrophilic nanoparticles, indicating that the viability of the cells is increased. Surface plasmon resonance (SPR) studies indicate that the hPGS coordinated FeOx-NP lead to an inhibition of L-selectin binding. Finally, the binding of hPGS functionalized FeOx-NP to myocarditis infected tissue is tested, using a mice-model. These results indicate that hPGS coordinated FeOx-NP may be suitable for being used as a contrast agent in magnetic resonance imaging.

CPP 2.12 Mon 12:45 C 243

Analysis of multivalent effects using single molecule force spectroscopy (SMFS) on pyridine coordination compounds — •Manuel Gensler[1], Christian Eidamshaus[2], Artur Galstyan[2], Ernst-Walter Knapp[2], Hans-Ulrich Reissig[2], and Jürgen P. Rabe[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin — [2]Institut für Chemie und Biochemie, Freie Universität Berlin

Multivalency is an important effect in biological processes and supramolecular assemblies. Multiple noncovalent interactions of two partners may occur with an affinity greater than the sum of the corresponding monovalent interactions. The mechanical stability of multivalent interactions is important for the understanding of numerous biological processes. However due to their complexity, the binding enhancement in such systems is not yet fully understood. [1]

We developed a simple model system using coordinative bonds between pyridine nanorods. SFM based single molecule force spectroscopy (SMFS) [2] in aqueous solutions of CuSO4, combined with DFT calculations of bond dissociation under force, revealed details of the bond opening that are usually not accessible by ensemble methods. The bivalent system rather opens successively than simultaneously, which leads to lower rupture forces than for the monovalent system, over a broad range of loading rates. Our model system can be varied to study structural effects influencing the mechanical stability of multivalent interactions.

[1] J.D. Badjic et al. Acc. Chem. Res. 2005, 38, 723-732. [2] M.I. Gianotti and G.J. Vancso ChemPhysChem 2007, 8, 2290-2307.

CPP 2.13 Mon 13:00 C 243

Mechanical Stability Behavior of Fullerenes — •Markus A. Hartmann[1], Melanie Todt[2], David Holec[3], Paul H. Mayrhofer[3], Oskar Paris[1], Franz D. Fischer[4], and Franz G. Rammerstorfer[2] — [1]Institute of Physics, Montanuniversitaet Leoben, Franz-Josef-Strasse 18, 8700 Leoben, Austria — [2]ILSB, Vienna University of Technology, Gusshausstrasse 27-29, 1040 Vienna, Austria — [3]Department of Physical Metallurgy and Materials Testing, Montanuniversitaet Leoben, Franz-Josef-Strasse 18, 8700 Leoben, Austria — [4]Institute of Mechanics, Montanuniversitaet Leoben, Franz-Josef-Strasse 18, 8700 Leoben, Austria

Carbon nanostructures are a fascinating class of materials combining high stiffness with low weight and exceptional toughness. Understanding the mechanical performance and stability of larger, hierarchical structures like carbon onions and fibers demands to understand the fullerene behavior also on microscopic length scales making a multi-scale/multi-method approach inevitable. We used ab initio calculations to extract classical potentials that were used in subsequent Monte Carlo simulations and Finite Element studies on larger structures. The simulations were used to perform (computational) mechanical tests on single fullerenes of different sizes to characterize their mechanical behavior. Special attention was paid to the influence of pentagons inherent in any fullerene structure on the stability behavior. The simulation results were compared to the predictions of Finite Element methods to evaluate macroscopic parameters like elastic modulus or Poisson ratio of the investigated structures.

CPP 3: Focus: Structural Ordering and Electronic Transport I (joint focus with HL)

As yet, there is no complete picture describing the influence of morphology on the transport of excitons and charge in organic semiconductors. This lack of understanding is in part due to the very complex and inhomogeneous morphology of these layers. This session aims to discuss the influence of molecular order, especially intramolecular and intermolecular order in crystalline and amorphous regions, on transport in conjugated molecular systems. Among other subjects, different model systems will be compared, ranging from ordered monolayers in UHV to macroscopic single crystals. (Organizers: Günter Reiter, Dieter Neher, Veit Wagner)

Time: Monday 9:30–13:15 Location: ER 270

Invited Talk CPP 3.1 Mon 9:30 ER 270

Neither crystalline nor amorphous: how charge transport is affected by order in organic semiconductors — •Alberto Salleo — Stanford University, Stanford, USA

From the fundamental standpoint, organic semiconductors are fascinating as they are neither crystalline nor amorphous and their microstructure plays a central role in governing charge transport. I will show that understanding disorder is the key to determining charge transport mechanism. Using advanced synchrotron-based X-ray characterization techniques we are able to define and measure structural order at different length-scales. We are particularly interested in cumulative disorder (paracrystallinity), where the lattice parameter takes on a Gaussian distribution about its mean value. The disorder parameter g allows us to rank materials quantitatively on a continuous scale, from a perfectly crystalline material ($g<1\%$) to an amorphous one ($g>10\%$). Using disorder as a ranking parameter, I will discuss the differences in transport between small molecule and polymer films as well as their respective inherent limitations and bottlenecks. This work may help devising design rules for new materials with desirable transport properties for polarons and excitons.

CPP 3.2 Mon 10:00 ER 270

Influence of Alkyl Side Chain Length on the Self-organization of RT and Low Temperature Cast Poly(3-alkylthiophene) Thin Films — •Shabi Thankaraj Salammal[1], Souren Grigorian[1], Ullrich Pietsch[1], Martin Brinkmann[2], Navaphun Kayunkid[2], Nils Koenen[3], and Ullrich Scherf[3] — [1]University of Siegen — [2]CNRS, Strasbourg — [3]University of Wuppertal

An enhancement of in-plane stacking of poly(3-alkylthiophene)s (P3ATs) with decrease of alkyl side chain length has been thoroughly analyzed using X-ray and electron diffraction (ED)technique. Thin films of poly(3-pentylthiophene), poly(3-hexylthiophene), poly(3-heptylthiophene), and poly(3-octylthiophene) (P3OT) were cast at 23°C(RT) and low (-30°C) temperature. Thin films prepared using the lowest concentration (1mg/14ml) envisages that the P3OT crystallites can provide highly edge-on oriented and bigger crystallites by casting at low temperature. The X-ray and electron diffraction patterns collected for the same films shows the poor in in-plane ordering of P3AT crystallites as the side chain length increases due to the augment in steric hindrance between the alkyl side chains. It subsequently reduces the photoluminescence (PL) efficiency as well as the field effect mobility of organic field effect transistors. The reduction in cast temperature together with the reduction of alkyl side chain length is resulting three distinct PL peaks with defined linewidths. The absence of face-on oriented crystallites while casting at -30°C can be explained by the prolongation of growth time caused by the reduced evaporation of solvent (Chloroform).

CPP 3.3 Mon 10:15 ER 270

Determination of the Crystallinity of Semicrystalline Poly(3-hexyl thiophene) by Means of Wide Angle X-Ray Scattering — •Jens Balko[1], Ruth Lohwasser[2], Michael Sommer[3], Mukundan Thelakkat[2], and Thomas Thurn-Albrecht[1] — [1]Institute of Physics, Martin-Luther-University Halle-Wittenberg, 06120 Halle — [2]Applied Functional Materials, Macromolecular Chemistry I, University of Bayreuth, 95440 Bayreuth — [3]Melville Laboratory for Polymer Synthesis, Department of Chemistry, University of Cambridge, Cambridge

Poly(3-hexyl thiophene) (P3HT) is a common polymer semiconductor, often used as material or component in organic field effect transistors or solar cells. The crystallinity of this semicrystalline material is among other parameters governing the electronic mobility. However, at present there is no routine method available to determine an absolute value for the crystallinity, and the values given in the literature e.g. for the enthalpy of melting vary by a factor of three. Wide Angle X-Ray Scattering (WAXS) probes the crystals as well the amorphous parts of the sample and there exists an established procedure to measure the crystallinity (RULAND, 1961) based on scattering data. The result is used for a reliable calibration of the melting enthalpy that can serve as a reference value for more convenient calorimetric techniques. We compare the crystallinity for a number of chemically well-defined samples, with different molecular weight and a typical commercial sample with broad molecular weight distribution. In addition, for some selected samples we study the influence of temperature on crystallinity.

CPP 3.4 Mon 10:30 ER 270

Formation of Single Crystals of Conjugated Polymers — •Khosrow Rahimi[1], Ioan Botiz[1,2], Natalie Stingelin[2,3], and Günter Reiter[1,2] — [1]Institute of Physics, University of Freiburg — [2]Freiburg Research Institute for Advanced Studies (FRIAS) — [3]Imperial College London

In order to improve optoelectronic properties of conjugated polymers, a profound understanding of the excitonic and electronic transport with respect to structure is crucial. By gaining a precise control over both molecular conformations and morphology we aim to obtain a correlation between orders at a macromolecular level to charge transport properties. The best controlled system for such a study is a single crystal which is free of grain boundaries and molecular disorder/defects.

Here, we report the preparation and structural properties of Poly(3-hexylthiophene) single-crystal grown by crystallization in dilute solutions. By employing a self-seeding approach, we were able to circumvent the nucleation process. To this end, we first dissolved all but a few small thermodynamically stable crystals, which then act as nuclei (seed crystals) for the subsequent crystallization step at higher polymer concentrations or at lower temperatures. This approach extends the accessible range for crystallization to lower degrees of supersaturation or supercooling. Using such conditions, we could control crystal size in all three dimensions as well as aspect ratio.

CPP 3.5 Mon 10:45 ER 270

Developing hybrid simulation schemes for mesoscale modeling of morphologies in organic semiconductors — •Kostas Daoulas[1,2], Victor Ruehle[1,3], and Kurt Kremer[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Innovation Lab GmbH, Heidelberg, Germany — [3]Department of Chemistry, University of Cambridge, United Kingdom

Hybrid simulations use a particle-based description while defining some interactions via collective variables. These degrees of freedom are soft; thus significant speedups of simulations are possible and large systems can be addressed. However, this softness of interactions poses challenges in modeling organic semiconductors where the local liquid structuring (e.g. pi-pi stacking) affects the mesoscale properties. As a first step in developing hybrid approaches incorporating this interplay, we consider here Monte Carlo simulations of homopolymer melts with nematic liquid-crystalline (LC) behavior. The polymers are described as discrete worm-like chains, a simple density functional controls the compressibility, and a functional of the local segmental orientation tensor captures the LC ordering. We illustrate that the method can address large systems parameterized according to volumetric and conformational properties representative of semiconductor materials by establishing a rough correspondence with regiorandom P3HT melts. Chain conformations and the effect of the molecular weight on the isotropic-nematic transition are studied. The formation of the nematic phase is addressed within the Rouse-like dynamics realized by the current model. We discuss directions of further methodological developments.

CPP 3.6 Mon 11:00 ER 270

Structure determination beyond crystallinity — •Chris Elschner[1], Sebastian Radke[2], Gianaurelio Cuniberti[2], Karl Leo[1], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik (IAPP), TU Dresden, 01069 Dresden, Germany — [2]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany

Organic semiconducting materials allow novel optoelectronic devices, combining the excellent optical properties of organic dyes with semiconductor behavior. Organic Light Emitting Diodes and Organic Solar Cells are successful examples in this field. Many organic materials grow strongly disordered or even amorphous in thin films. To distinguish between crystalline or amorphous thin films, X-ray diffraction measurements can be used. If Bragg reflections are missing, organic films are simply classified as amorphous in literature without any specification. We show that it is possible to extract short range order informations even from amorphous organic layers. Using a special grazing incidence X-ray diffraction method [1] it is possible to measure the diffuse scattering of amorphous DBP organic layers. A structural model of the short range order within a few nm gives insight of the molecular stacking in the amorphous layer. The structural model is used as starting configuration for mobility calculations based on Monte Carlo simulations. Finally, the correlation between short range molecule stacking and charge transport is investigated.

[1] C. Elschner et al. Journal of Applied Crystallography 44, 983-990(2011).

30 min break: Possibility for discussions

Invited Talk CPP 3.7 Mon 11:45 ER 270

Charge transport and recombination in organic light-emitting diodes — •Paul Blom — TNO Holst Centre, Eindhoven, Netherlands

Charge transport and charge recombination are recognized as key ingredients in the performance of polymer light emitting diodes (PLEDs). We observe that in conjugated polymers the electron transport is limited by traps that are Gaussianly distributed in energy within the band gap. Remarkably, we show that the electron trap distribution is identical for a large variety of polymers, hinting at a common origin for electron traps. Photogenerated current measurements on PLED device structures reveal that next to the known Langevin recombination also trap-assisted recombination is an important recombination channel in PLEDs. The dependence of the open-circuit voltage on light intensity enables us to determine the strength of this process. Numerical modeling of the current-voltage characteristics incorporating both Langevin and trap-assisted recombination yields a correct and consistent description of the PLED, without the traditional correction of the Langevin pre-factor. At low bias voltage the trap-assisted recombination rate is found to be dominant over the free carrier recombination rate. As a result, we show that the ideality factor in the diffusion regime of a bipolar diode is governed by the recombination of trapped electrons with free holes.

CPP 3.8 Mon 12:15 ER 270

Investigations of charge generation, transport and recombination on organic solar cells based on merocyanines — •Steven Graf[1], Vera Steinmann[1], Nils Kronenberg[1], Martin Lenze[1], Dirk Hertel[1], Frank Würthner[2], and Klaus Meerholz[1] — [1]Institut für Physikalische Chemie, Universität zu Köln, Luxemburger Str. 116, 50939 Köln (Germany) — [2]Institut für Organische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg

Organic photovoltaics offer a very promising green energy alternative. Highly efficient organic solar cells can be produced by cost-effective methods such as coating from solution (SOL) or depositing under high vacuum conditions (VAC).

We investigate merocyanines (MC), a class of low-molecular-weight colorants, as donor material in organic solar cells. These molecules are processable via both deposition techniques, showing remarkable power conversion efficiencies (PCE) beyond 4% for SOL- and 6% for VAC-processed devices.

Towards even higher PCEs it is imperative to gain a better understanding of the fundamental processes of charge carrier generation, transport and recombination in MC solar cells. We carried out a detailed study of these processes using steady- state and time-resolved photoluminescence spectroscopy and current-voltage measurements. The influence of morphology on fundamental processes is elucidated by varying the deposition conditions as well as the fabrication method. The investigations are supported by temperature- and electric-field-dependent studies of charge recombination and transport.

CPP 3.9 Mon 12:30 ER 270

Morphology triggered impact of charge carrier recombination on the current–voltage response of organic solar cells — •Alexander Foertig[1], Markus Gluecker[1], Alexander Wagenpfahl[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius-Maximilians-University of Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Bavarian Centre for Applied Energy Research (ZAE Bayern e.V.), Am Hubland, 97074 Würzburg, Germany

In view of a commercialization the efficiency of organic solar cells still has to be improved. Therefor a proper understanding of the fundamental physical processes is required. The non-geminate loss mechanisms of photo-generated charges in polymer:fullerene bulk heterojunction solar cells are studied using the complementary measurement techniques charge extraction (CE), transient photovoltage (TPV) and transient photocurrent (TPC). From voltage dependent charge carrier densities $n(V)$ a loss current $j_{loss}(V)$ can be determined. For systems predominately based on a voltage independent charge photo-generation this analysis successfully allows to reconstruct the measured I/V response. Devices based on the promising copolymer PTB7 blended with $PC_{71}BM$ are used to study the influence of morphology on the recombination dynamics and thus the I/V characteristics. Furthermore we applied macroscopic device simulations to analyse the influence of the spatial distribution of charges in the active layer which can not be accounted for in the experiment.

CPP 3.10 Mon 12:45 ER 270

Temperature and carrier concentration dependent analysis of charge transport in Poly (3-hexylthiophene) based organic field effect transistors — •Hippolyte Hirwa and Veit Wagner — School of Engineering and Science Jacobs University Bremen Campusring 1, D-28759 Bremen (Germany)

A crucial step of organic electronics towards applications is the understanding and exploiting of their charge transport mechanisms. Several models have been previously developed in order to explain the behavior of organic semiconductors. These proposed models (e.g. Vissenberg Matters model, multiple trapping and release model and Neldel Meyer rule) try to include effects like temperature dependence, charge carrier concentration dependence and field dependence. However, these models can not fully explain our experimental data obtained on P3HT based organic field effect transistors manufactured on flexible PET foils. The Neldel Meyer rule hardly showed agreement with our experimental data. The Vissenberg and Matters model and the multiple trapping and release model showed a good agreement but only over a limited temperature range. For temperatures below 170K an additional transport mechanism is observed which is explained by a modification of the Vissenberg and Matters model.

CPP 3.11 Mon 13:00 ER 270

Morphology controlled charge transport in diblock copolymer based solar cells — •Chetan Raj Singh[1], Ruth Lohwasser[2], Olesia Synooka[1], Mukundan Thelakkat[2], Gerhard Gobsch[1], and Harald Hoppe[1] — [1]Institute of Physics, TU Ilmenau, Germany — [2]Applied Functional Polymers, University of Bayreuth, Germany

The block copolymers as an active material have been sought after in solar cells to realize scalable and morphologically stable polymer solar cells. We report here the charge carrier mobilities of holes and electrons in the studied diblock copolymer (P3HT-b-PPerAcr) and in its constituting homopolymers, P3HT and PPerAcr. We discuss the effects of charge carrier mobility imbalance and its consequence on solar cell properties. In the study, the morphology of the diblock copolymer is altered by blending donor component and subsequent thermal treatments which have given rise to up to two orders of magnitude increase in charge carrier mobilities. Furthermore, the influence of morphology and achieved charge carrier mobility balance are studied on solar cell devices.

CPP 4: Glasses I (joint session with DY)

Time: Monday 15:00–17:30 Location: C 243

Invited Talk CPP 4.1 Mon 15:00 C 243

Glass transition by molecular network topology freezing and discovery of vitrimers — •Ludwik Leibler, Damien Montarnal, Mathieu Capelot, and François Tournilhac — Matière Molle et Chimie, ESPCI, 10, rue Vauquelin, 75005 Paris, France

We will discuss a concept and practical realizations of a glass transition by reversible topology freezing of a molecular network. Permanently cross-linked materials, like thermosets or rubbers, have outstanding mechanical properties and solvent resistance, but they cannot be processed and reshaped once synthesized. Non-cross-linked polymers and those with reversible cross-links are processable, but they are soluble. We design epoxy networks able to rearrange their topology by exchange reactions without depolymerization and show that they are insoluble and processable. Unlike organic compounds and polymers whose viscosity varies abruptly near glass transition, these networks, vitrimers, show Arrhenius-like gradual viscosity variations just like vitreous silica. Like silica, the vitrimers can be wrought and welded to make complex objects by local heating without the use of molds. The concept of a glass, made by reversible topology freezing in epoxy networks can be readily scaled up for applications and generalized to other chemistries.

Topical Talk CPP 4.2 Mon 15:30 C 243

Elastic Properties of 2D amorphous solids — •Peter Keim — Universität Konstanz

Using positional data from video-microscopy of a two-dimensional colloidal system and from simulations of hard discs we determine the wave-vector-dependent normal mode spring constants in the supercooled fluid and glassy state, respectively. The emergence of rigidity and the existence of a displacement field in amorphous solids is clarified. Continuum elastic theory is used in the limit of long wavelengths to analyze the bulk and shear modulus of this amorphous system as a function of temperature. The onset of a finite static shear modulus upon cooling marks the fluid/solid transition. This provides an opportunity to determine the glass transition temperature T_G in an intuitive and precise way.

CPP 4.3 Mon 16:00 C 243

Heterogeneous shear in hard sphere glasses — •Fathollah Varnik[1,2], Suvendu Mandal[2], and Dierk Raabe[2] — [1]ICAMS, Ruhr University Bochum, Germany — [2]Max-Planck-Institut fuer Eisenforschung, Duesseldorf, Germany

There is growing evidence that the flow of driven amorphous solids is not homogeneous, even if the macroscopic stress is constant across the system [1,2]. Via event driven molecular dynamics simulations of a hard-sphere glass, we provide first direct evidence for a correlation between the fluctuations of the local volume-fraction and the fluctuations of the local shear rate [3]. Higher shear rates do preferentially occur at regions of lower density and vice versa. The temporal behavior of fluctuations is governed by a characteristic time scale, which, when measured in units of strain, is independent of shear rate in the investigated range. Interestingly, the correlation volume is also roughly constant for the same range of shear rates. A possible connection between these two observations is discussed.

[1] F. Varnik, L. Bocquet, J.-L. Barrat, L. Berthier, Phys. Rev. Lett. 90, 095702 (2003).

[2] R. Besseling, L. Isa, P. Ballesta, G. Petekidis, M.E. Cates, W.C.K. Poon, Phys. Rev. Lett. 105, 268301 (2010).

[3] S. Mandal, M. Gross, D. Raabe, F. Varnik, submitted to Phys. Rev. Lett.

CPP 4.4 Mon 16:15 C 243

Effect of cross-link density on re-entrant melting of microgel colloids — •Malte Wiemann[1], Norbert Willenbacher[2], and Eckhard Bartsch[1,3] — [1]University of Freiburg, Department of Physical Chemistry, Freiburg, Germany — [2]Karlsruhe Institute of Technology, Department of Mechanical Process Engineering and Mechanics, Karlsruhe, Germany — [3]University of Freiburg, Department of Macromolecular Chemistry, Freiburg, Germany

Fluid states of colloidal dispersions at volume fractions above the glass transition can be accessed by introducing short-ranged depletion attraction [1]. For a binary mixture of PS-microgel particles (crosslinking density 1:50) in a good organic solvent DLS-measurements revealed a fluidization up to a volume fraction ϕ=0.69 when linear nonadsorbing polymer is added. The high packing fraction up to which fluid states could be observed raised the question whether the magnitude of this effect is a specialty of the microgel system. We prepared microgels with a much higher crosslinking density (1:10) which should be a good approximation of hard sphere colloids. Fluid states could again be obtained above ϕg, however, up to a significantly smaller packing fraction. The amount of free polymer needed to fluidize the dispersion was much lower as compared to the previous mixture [2]. The existence of fluid states up to high volume fractions for the 1:50 crosslinked particles is - at least partially - a microgel effect which is at present not fully understood and possible origins will be discussed. [1] K. Dawson etal., Phys. Rev. E 63, 011401 (2000) [2] M. Wiemann, N. Willenbacher, E. Bartsch, Colloid Surface A, 10.1016/j.colsurfa.2011.11.029

CPP 4.5 Mon 16:30 C 243

Epoxy resins in confined geometry — •Anna Silex, Jörg Baller, and Roland Sanctuary — Laboratory of Physics of Condensed Matter and Advanced Materials, University of Luxembourg, 162A, Avenue de la Faiencerie, L-1511 Luxembourg

In order to exemplarily study the influence of confinement on the behavior of a widely used epoxy resin (Diglycidil Ether of Bisphenol A, DGEBA), we have filled mesoporous glasses with different pore radii with the low molecular weight liquid. Several confinement effects are known to take influence on the glass transition of small molecule liquids. Firstly, interactions between the glass former and the large internal surface of the porous glass lead to a slowing down of the molecular dynamics. Secondly, the confinement of the liquid molecules by the pores and the layer is generally known to accelerate the molecular dynamics. Finally, negative pressure building up in the pores due to the mismatching thermal expansion coefficients of the liquid and the porous glass is discussed to lead to a lower glass transition temperature compared to the pure materials. We present experimental results obtained for DGEBA-porous glass systems with stochastically modulated calorimetry and thermo-mechanical analysis. Thereby the focus is on the influence of the pore size on the glass transition behavior of the guest material but also on the macroscopic characteristics of the complete system as a result of the confinement. Differences between the thermal expansion of the empty and DGEBA filled samples are highlighted.

CPP 4.6 Mon 16:45 C 243

Glassy dynamics of isolated polymer coils — •Martin Tress, Emmanuel Mapesa, and Friedrich Kremer — Universität Leipzig, Leipzig

For the first time, the glassy dynamics of randomly distributed, isolated poly(2-vinylpyridine) (P2VP) polymer coils is studied by means of Broadband Dielectric Spectroscopy (BDS). This is achieved by recently developed nano-structured electrode arrangements where isolated polymer coils are deposited onto ultra-flat, highly conductive silicon electrodes. Atomic Force Microscopy scans of the identical sample before and after the BDS measurement prove that the volume of the coils matches, within a factor of 10 (reflecting the broad molecular weight distribution), with the expected volume of a single chain (considering bulk density and the respective molecular weight). The observed dynamics compares well with that of bulk but is slowed down by a factor of about 10. This is attributed to attractive interactions of the P2VP segments with the supporting silica surface.

CPP 4.7 Mon 17:00 C 243

Reduced Glass Transition Temperatures of Thin Polymer Films - Confinement Effect or Artifact? — •Oliver Bäumchen[1], Joshua D. McGraw[1], James A. Forrest[2], and Kari Dalnoki-Veress[1] — [1]Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, L8S 4M1 — [2]Department of Physics and Astronomy and Guelph-Waterloo Physics Institute, University of Waterloo, Waterloo, ON, Canada, N2L 3G1

For two decades there have been reports of measurements of reduced glass transition temperatures (T_g) in polymer, and in particular polystyrene, films. These results have motivated theoretical models and a variety of sophisticated experiments probing interfacial polymer properties. While the much larger reductions in T_g for free standing films have suggested the importance of the free surface, a significant concern has been raised about a possible correlation between anomalous dynamics and incomplete equilibration of the sample. Here, we present new ellipsometry measurements which unambiguously address this concern. The glass transition in free standing and supported films can be changed by many 10's of degrees by manipulating the interfacial properties. Taken together with previous work the results clearly reveal the importance of free interfaces as we transition from two, to one, to zero free interfaces.

CPP 4.8 Mon 17:15 C 243

Molecular Mobility and Glass Transition of Thin Poly(Bisphenol A Carbonate) Films — •Huajie Yin and Andreas Schönhals — BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany

Glass transition behavior of thin poly(bisphenol A carbonate) (PBAC) films (down to 10 nm) was investigated using capacitive dilatometry (CD), broadband dielectric spectroscopy (BDS) and differential ac-chip calorimeter (DACC) accompanied by contact angle measurements. In the BDS measurements of the thin PBAC films capped between two Al layers, no thickness dependence of the segmental dynamics was detected down to a critical thickness of 20 nm. For thickness below 20 nm, an increase of the relaxation time at a fixed temperature was observed. The thickness dependence of the thermal glass transition temperature determined by CD is in agreement with BDS results. Dynamic glass transition temperature of the ultra-thin PBAC films (10-55 nm) supported on SiO2 layer, with one free surface, was studied by means of differential ac-chip calorimeter as well. No thickness dependence of the dynamic glass transition temperature was observed within an uncertainty of +/-3 K for each frequency. These experimental results are discussed in terms of the different interactions of polycarbonate segments with the different substrates and/or different preparation conditions.

CPP 5: Focus: Structural Ordering and Electronic Transport II (joint focus with HL)

Time: Monday 15:00–17:30 Location: ER 270

Invited Talk CPP 5.1 Mon 15:00 ER 270

Single-Molecule Spectroscopy of Conjugated Polymers: Unravelling Chain Conformations from the Bottom Up — •John Lupton — Institut für Experimentelle und Angewandte Physik, Universität Regensburg — Department of Physics and Astronomy, University of Utah, Salt Lake City

When considering molecular morphology in the context of plastic electronics, one usually refers to the level of intermolecular order. Yet because of the large molecular weight and the interplay between intrinsically flexible and stiff molecular bonds, intramolecular morphology is crucial in determining the overall macroscopic properties of a material. Single-molecule fluorescence spectroscopy offers a unique approach to quantifying intrachain order and disorder, rigidity and shape, and the respective influence on electronic structure so as to construct a microscopic understanding of a functional material from the bottom up. Examples where the technique has proven particularly successful include polyfluorene, which can display a wide range of intrachain conformations including the extraordinary case of perfect defect-free pi-chains; and in polyhexylthiophene, which exhibits a uniquely broad range of conjugation lengths which can be directly mapped on the single-chain level.

CPP 5.2 Mon 15:30 ER 270

Rod-coil transitions in the polymers MEH-PPV and PFO — •Anna Köhler — Universität Bayreuth, Bayreuth, Germany

In the current work we explore the effect of aggregation of three conjugated polymers, MEH-PPV , PFO and MeLPPP, dissolved in MeTHF. In MEH-PPV, the absorption spectra are a superposition of a broad ("blue") band and a vibrationally well resolved spectrum at lower energies (the "red"-phase)that appears at 190 K and grows at the expense of the blue phase. Obviously there is a temperature-induced transformation from the blue to the red phase. While this is observed in solutions of 5 x 10-6 mol/L , the red-phase is absent in a 10-7 mol/L solution. This proves that the formation of the red-phase requires aggregation. A similarly temperature dependent superposition of blue and red features can also observed for PFO, but upon dilution only the red feature survives. Finally for MeLPPP, the absorption and fluorescence spectra are mono-modal at all temperatures.The results are indicative of a rod-coil transition in the case of MEH-PPV and PFO with a temperature dependence that is characteristic of a order-disorder transition, albeit with different driving forces. In the case of

MEH-PPV the planarization of the chain requires chain aggregation. Quantum chemical calculations show the potential for torsional motion of the repeat units is so shallow that the motion the solvent molecules above the glass temperature is sufficient to prevent chain elongation unless chain pairing occurs. In PFO, however, the tendency towards chain planarization is obviously strong enough to facilitate the elongation of single chains and inter-chain interaction obstructs rather than helps chain elongation.

CPP 5.3 Mon 15:45 ER 270

Aggregation in a High Mobility n-type Low Bandgap Copolymer: Implications on Morphology and Charge Transport — ●Robert Steyrleuthner[1], Marcel Schubert[1], Ian Howard[2], Christian Schilling[3], Bastian Klaumünzer[4], Zhihua Chen[5], Peter Saalfrank[4], Frederique Laquai[2], Antonio Facchetti[5], and Dieter Neher[1] — [1]University of Potsdam, Institute of Physics — [2]MPI for Polymer Research, Mainz — [3]Nanolytics GmbH, Potsdam — [4]University of Potsdam, Institute of Chemistry — [5]Polyera Corporation, Illinois

The prominent copolymer P(NDI2OD-T2) exhibits very high electron OFET mobility of 0.85 cm2/Vs. Recent X-ray studies on P(NDI2OD-T2) revealed an exceptional in-plane order with distinct pi-stacking of the NDI cores (Rivnay et al.) while GIXD and NEXAFS measurements suggested a significant fraction of amorphous content (Schuettfort et al.). By investigating steady state and time dependent UV-Vis absorption/fluorescence spectroscopy on solutions of P(NDI2OD-T2), we identified distinct absorbing species and assigned them to intrachain CT-excitons on disorderd chains and to interchain excitations on aggregated chains. These results were confirmed by DFT calculations on individual and stacked chains. Analytical ultracentrifugation showed that aggregation in solution proceeds via the collapse of individual polymer coils. The analysis of chain aggregation in solution allowed for the quantitative deconvolution of the thin film absorption, yielding the aggregate content. Finally we find that the vertical transport (electron-only devices) is largely affected by the layer crystallinity.

CPP 5.4 Mon 16:00 ER 270

Probing Exciton and Charge Dynamics in Low-Bandgap Polymer:Fullerene Blends by NIR Transient Absorption Spectroscopy — Ian Howard, Fabian Etzold, Clare Dyer-Smith, Hannah Mangold, Ralf Mauer, Michael Meister, and ●Frédéric Laquai — Max Planck Research Group for Organic Optoelectronics, Max Planck Institute for Polymer Research Mainz, Germany

Low-bandgap polymers are among the most promising donor materials for bulk heterojunction organic solar cells with efficiencies now exceeding 7 %. However, the photophysics of the pristine polymers and the mechanisms of charge generation and recombination in low-bandgap polymer:fullerene blends are still not entirely understood. In this contribution we compare the exciton and charge carrier dynamics of relevant low-bandgap polymers including PCDTBT, PCPDTBT and PTB-type polymers and their photovoltaic blends, which we study by broadband transient absorption (TA) spectroscopy covering a dynamic range from femto- to milliseconds. We present the previously unobserved near-infrared (NIR) spectral range up to 2000 nm, which we observe with our recently developed broadband NIR-TA setup. We show that by detecting the NIR spectral range we are able to distinguish between the spectral features of singlet and triplet excitons as well as charge-transfer states and mobile polarons and that we can study their generation and decay dynamics, which is difficult, if not impossible, by conventional broadband visible transient absorption spectroscopy.

Invited Talk CPP 5.5 Mon 16:15 ER 270

Band dispersion and localized states in organic solids — Nobuo Ueno[1] and ●Norbert Koch[2] — [1]Graduate School of Advanced Integration Science, Chiba University, Chiba, Japan — [2]Institut f. Physik, Humboldt-Universität zu Berlin, Berlin, Germany

Charge transport in solids is inevitably linked with structural properties. Organic molecular materials are characterized by two hierarchical levels of structure, i.e., the structure of an individual molecule and that of the molecular assembly. As a consequence, both affect the organic solid's electron density of states (DOS) and the mechanisms of charge transport. We give an overview of how photoelectron spectroscopy can be used to study the DOS of organic materials ranging from amorphous thin films to single crystals, and how the sample's structure (including defects) is reflected in localized (gap) states or delocalized dispersing bands. The influence of the molecular chemical structure and the dielectric environment on electron-vibron coupling strength will be discussed. We will address the impact of polymorphism and temperature on the band structure of prototypical organic solids, including tetracene, pentacene, and rubrene.

CPP 5.6 Mon 16:45 ER 270

Elucidating excitonic coupling in supramolecular dye nanotubes — ●Dorthe M. Eisele[1], Dylan H. Arias[1], Colby P. Steiner[1], Robert J. Silbey[1], Xiaofeng Fu[2], Daniela Nicastro[2], Keith A. Nelson[1], and Moungi G. Bawendi[1] — [1]MIT, USA — [2]Brandeis University, USA

Self-assembled molecular nanotubes, in particular those strongly absorbing visible light, are highly promising quasi-1d systems for opto-electronic and light harvesting (LH) applications. A detailed understanding of the energetics, dynamics, and couplings of excitonic states in these nanoscale systems is the key for further development of such applications. We report on a remarkable example of such a system, i.e., well-defined nanotubular aggregates of amphiphilic cyanine dyes [1]. By means of cryogenic electron microscopy and 2d electronic spectroscopy, we show that excitonic interactions in such nanoscale systems are not only highly sensitive to changes within the supramolecular structure, but also to changes in higher ordering [2]. This addresses the fundamental question of what physical properties control the energy transport processes in excitonic nanoscale systems, which are vital for new developments in opto-electronic applications.

[1] D.M. Eisele, *et al.*, Nature Nanotech. 4 (2009); D.M. Eisele, *et al.*, JACS Comm. 132 (2010); D.M. Eisele, C.M. Cone, E.A. Bloemsma, S.M. Vlaming, R.J. Silbey, M.G. Bawendi, J. Knoester, J.P. Rabe, and D.A. Vanden Bout (submitted);[2] D.M. Eisele, D.H. Arias, C.P. Steiner, X. Fu, D. Nicastro, K.A. Nelson, and M.G. Bawendi (to be submitted)

CPP 5.7 Mon 17:00 ER 270

Intermolecular torsional motion of a π-aggregated dimer probed by two dimensional spectroscopy — ●Joachim Seibt[1] and Alexander Eisfeld[1,2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden — [2]Department of Chemistry and Chemical Biology Harvard University, 12 Oxford Street, Cambridge, MA 02138

The energetic splitting of the two exciton states of a molecular dimer depends strongly on the relative orientation of the monomers with respect to each other. The curvature of the corresponding adiabatic potential energy surfaces can lead to torsional motion of the monomers. It has been suggested recently that this torsional motion could provide a possible relaxation mechanism for the upper state which proceeds via a crossing of the two excited state potentials. Another, competing, relaxation mechanism is provided by coupling to the environment, leading to direct exciton relaxation. Here we examine theoretically the combined dynamics of torsional motion and excitonic relaxation for a π-aggregated dimer. Using two dimensional (2D) spectroscopy it is shown how torsional motion through a crossing of the adiabatic excitonic potential surfaces could be distinguished from direct relaxation. For the calculations a mixed quantum/classical approach is used, where the torsional motion is treated by an Ehrenfest type of equation, while the excitonic dynamics including dephasing and direct relaxation is described by a quantum master equation.

CPP 5.8 Mon 17:15 ER 270

Origins of low charge mobility in crystalline acceptor-substituted oligothiophenes — Manuel Schrader[1], Roland Fitzner[2], Moritz Hein[3], Chris Elschner[3], Bjoern Baumeier[1], Moritz Riede[3], Karl Leo[3], and ●Denis Andrienko[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Institute of Organic Chemistry II and Advanced Materials, Ulm, Germany — [3]Institute of Applied Photophysics, Dresden, Germany

In a small molecule-based organic solar cell, optical absorption in the visible spectrum, needed for efficient photon harvesting, and the relative donor-acceptor level alignment, required for efficient exciton dissociation, are currently achieved by tuning the electron affinity, the ionization potential, and the band gap of the donor material. In dicyanovinyl-substituted oligothiophenes this is realized by covalently binding an electron-withdrawing group (dicyanovinyl) to an electron-donating core (thiophene oligomer). Such an internal donor-acceptor molecular architecture, however, results in large local molecular dipole moments and thus substantial electrostatic energetic disorder, which leads to pronounced Poole-Frenkel behavior and low charge mobilities, even in a crystalline phase. Analyzing charge transport of dicyanovinyl-substituted oligothiophenes, we propose chemical design rules for the donor which offer a compromise between band gap and charge mobility engineering.

CPP 6: Poster: Structural Ordering and Electronic Transport (joint focus with HL)

Time: Monday 17:30–19:30 Location: Poster A

CPP 6.1 Mon 17:30 Poster A

Multiscale molecular simulations of P3HT:PCBM blends — •Olga Guskova[1], Andreas John[1], Peter Friedel[1], and Jens-Uwe Sommer[1,2] — [1]Leibniz Institute of Polymer Research, Dresden, Germany — [2]TU Dresden, Dresden, Germany

We apply a multi-level approach including micro- and mesoscale simulation to investigate the nanoscale morphologies of bulk heterojunction blend films comprising poly(3-hexylthiophene) (P3HT) and the methanofullerene derivative phenyl-C61-butyric acid methyl ester (PCBM). DFT provides the information about local system morphology and the electronic properties that are important for device performance. Full-atomistic MD simulations expand the accessible length and time scale to ranges of heterojunction regions. Combination of these methods provides a deeper insight into the relations between structural and electronic properties of polymer-based donor/acceptor materials. Since existing force-fields do not properly reproduce the torsion angle between neighboring thiophene rings, we optimized dihedral angle potential between neighboring thiophene rings and validated the empirical force field PCFF for PCBM and P3HT. Simulations of blended P3HT and PCBM molecules were carried out to study the conformations at the P3HT/PCBM interface which crucial to our understanding of both the morphology evolution of the active layer in photovoltaic devices and charge separation/recombination rules. Since morphology has a direct impact on the electronic properties of the device, DFT studies of the realistic morphologies, based on MD simulations, enables a more accurate prediction of the device performance.

CPP 6.2 Mon 17:30 Poster A

Distribution of States and Energetic Disorder in P3HT:PCBM Blends — •Ilja Lange, Juliane Kniepert, Peter Brückner, James C. Blakesley, and Dieter Neher — University of Potsdam

P3HT:PCBM has been widely used as a promising candidate for research on organic photovoltaic because of its relatively high efficiency of 3-5%. However, this system is still not fully understood and some basic fundamental processes are still lacking. One reason for this incomplete picture is the lack of information about the energetic landscape of these devices. Established techniques like photoemission spectroscopy or cyclic voltammetry only deliver a rough approximation of the position of relevant transport bands and states. Instead, exact information about the distribution of states and their broadening is preferable for a comprehensive insight into e.g. open-circuit voltage, charge carrier generation, recombination and extraction.

Recently, we showed that charge injection into the low densities of tail states of organic semiconductors can be detected sensitively by Kelvin Probe [1]. By careful numerical analysis of the measurements, the distribution of tail states can be quantified. Here we apply this technique to explore the energetic structure of P3HT:PCBM blends. Surprisingly, we find that the energetic structure of both the donor and acceptor components change dramatically upon thermal treatment. These results open up interesting new insights into fundamental processes of this popular material system that have wider implications for all organic solar cells.

[1]Phys. Rev. Lett. 106, 216402 (2011)

CPP 6.3 Mon 17:30 Poster A

Recombination process in organic photovoltaic solar cells based on BTD/DPP copolymers studied by IV-characteristics — •Olesia Synooka — Physics institute,TU Ilmenau, 98693 Ilmenau, Germany

The short-circuit current density (Jsc) of polymer/fullerene bulk heterojunction solar cells based on benzothiadiazole (BTD) and/or diketopyrrolopyrrole (DPP) is investigated as a function of light intensity. The influence of light intensity and recombination strength on Jsc is consistently explained by a model based on the notion that the quasi-Fermi levels are constant throughout the device, including both drift and diffusion of charge carriers. A typical feature of polymer/fullerene based solar cells is that Jsc does not scale exactly linearly with light intensity (I). Instead, a power law relationship is found given by Jsc(Ia), where a ranges from 0.7 to 0.8. In a number of reports this deviation from unity is attributed to the occurrence of bimolecular recombination. Here is demonstrated the model calculations which shows that bimolecular recombination leads not a 100% of a typical loss of all free charge carriers at Jsc for these devices but it also governed by the build-up of space charge in the device.

CPP 6.4 Mon 17:30 Poster A

Influence of different organic ligands on the charge transport and charge transfer characteristics of CuInS2/polymer hybrid mixtures — •Christopher Krause, Nikolay Radychev, Florian Witt, Marta Kruszynska, Dorothea Scheunemann, Joanna Kolny-Olesiak, Holger Borchert, and Jürgen Parisi — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, 26111 Oldenburg

CuInS2 (CIS) nanoparticles embedded into a conductive polymer are a promising candidate for hybrid photovoltaic application due to unique features of the CIS nanomaterials. One of the key problems of the hybrid solar cells functionality is the creation of an efficient bulk heterojunction itself. In most cases, nanoparticles in the polymer matrix have to be stabilized by organic ligands, which can impede efficient charge transport through the hybrid blends as well as charge separation at the polymer/nanoparticle interface. Therefore an exchange of the initial ligand is required and might significantly improve the performance of semiconductor nanoparticle based hybrid solar cells. In the present work, the influence of different organic ligands on the charge transport in CIS and CIS/polymer blends is investigated by current-voltage measurements in a device geometry similar to solar cells and compared to mobility measurements in organic field-effect transistors (OFETs). Additionally, the charge transfer process at the donor/acceptor interface is studied by electron spin resonance.

CPP 6.5 Mon 17:30 Poster A

Subsurface imaging of P3HT:PCBM blends — •Martin Dehnert[1], Mario Zerson[1], Sven Hüttner[2], Zhuxia Rong[2], Ullrich Steiner[2], and Robert Magerle[1] — [1]Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Chemnitz, Germany — [2]Cavendish Laboratory, JJ Thomson Avenue, Cambridge, U.K.

We investigate the surface morphology of thin films of poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl C61-butyric acid methyl ester (PCBM) blends using AFM based amplitude-phase-distance-curves (APD). We use the indentation of the tip into the soft surface layer to measure the mechanical properties as a function of the tip indentation which allows reconstructing three dimensional depth profiles of the top 10 nm of the film. We show surface depth profiles of blends with varying ratio of P3HT:PCBM and study structural changes after different thermal annealing steps. The soft amorphous layer on the surface are formed to be between five and ten nanometers thick. We discuss the impact of the surface morphology and the amorphous top layer on the efficiency of organic solar cells.

CPP 6.6 Mon 17:30 Poster A

Ordered TiO2 single crystal nanowire arrays for hybrid solar cells — •Julian Reindl[1], Jonas Weickert[1], Andreas Wisnet[1], Christina Scheu[1], and Lukas Schmidt-Mende[2] — [1]Ludwig-Maximilians-University, Munich — [2]University of Konstanz

Organic Solar cells are an interesting technology where remarkable efficiencies beyond 8 % have been realized with the bulk heterojunction concept. Here a donor-acceptor blend is fabricated as absorbing and charge transporting layer. Even though this concept is striking for thin films, the unordered inner morphology of the active layer has detrimental effects in thicker layers due to higher charge trapping and charge carrier recombination. A promising approach to realize thicker active layers with accordingly higher absorptivity is the hybrid solar cell concept, where the organic donor is substituted by a wide band gap metal oxide like titania (TiO2). The TiO2 can be nanostructured, resulting in a controlled phase separation of donor and acceptor.

Here we present a possibility of synthesizing a layer of ordered monocrystaline rutile titania wires with controllable properties such as wire length, diameter and spacing. This layer acts as electron transporting matrix and should provide enhanced electron mobility compared to polycrystaline titania layers. In order to fabricate hybrid solar cells we fill these structures with the commonly used polymer P3HT. For better structure filling novel attempts using different methods are studied, including interface engineering and an approach using diethylflourene monomers, which can be polymerized inside the structure.

CPP 6.7 Mon 17:30 Poster A

Nanostructured Hybrid Solar Cells — •Jonas Weickert[1,2], Andreas Wisnet[1], Christina Scheu[1], and Lukas Schmidt-Mende[2] — [1]Ludwig-Maximilians-University Munich, Munich, Germany — [2]University of Konstanz, Konstanz, Germany

Organic solar cells have gained remarkable interest during the past two decades and have reached high power conversion efficiencies of 8%. However, efficiencies are still limited by relatively low absorptivity. Only thicker active layers could allow more complete photon harvesting. However, the active layer thickness of conventional organic solar cells is conceptually limited due to the relatively uncontrolled morphology of their active layers, which promotes charge carrier recombination for films thicker than 100-200 nm.

One way to overcome these limitations is the substitution of the organic acceptor material with wide band-gap semiconductors like TiO2 in so-called hybrid solar cells. TiO2 also acts as electron acceptor but can be nanostructured in order to meet the competing demands of high interfacial area and consistent pathways for charge transport.

TiO2 nanotubular arrays with dimensions comparable to exciton diffusion lengths in typical organic materials are synthesized on conductive glass substrates via electrochemical anodization of thin Ti films and can be readily infiltrated with donor material to realize ordered hybrid heterojunctions.

The properties of the metal oxide-organic junction can be further tuned by introduction of interfacial modifiers like dye molecules and are investigated in detail.

CPP 6.8 Mon 17:30 Poster A

Solvent additives for tuning the photovoltaic properties of polymer-fullerene solar cells — •Anna Göritz[1], Antonietta De Sio[2], Thomas Madena[2], Ralph Huber[2], Jürgen Parisi[2], Shany Neyshtadt[3], Felix Deschler[3], Enrico Da Como[3], Salvatore Esposito[4], and Elizabeth von Hauff[1,2] — [1]Physics Institute, University of Freiburg — [2]Physics Institute, University of Oldenburg — [3]Dep. of Physics and CeNS, LMU, Munich — [4]ENEA Research Center, Localita Granatello, Portici, Italy

We demonstrate that using solvent additives to prepare P3HT:PCBM blends increases the performance of bulk heterojunction solar cells by inducing favorable phase segregation and increased polymer ordering in the active layer[a]. The solvent additives 1,2,3,4-tetrahydronaphtalene (THN) and chlorobenzene were added to the host solvent 1,2-dichlorobenzene (oDCB) to influence the film formation properties. Solar cells prepared using solvent additives resulted in higher photocurrents than solar cells prepared using pure oDCB, and blends prepared from THN resulted in best efficiencies. Structural investigations with TEM, AFM, and Kelvin probe force microscopy indicated that the solvent additives lead to preferential in-plane phase segregation between the polymer and fullerene and increased P3HT ordering in the blends. The solvent additives led to a decrease in the PCBM content at the top of the blend, resulting in lower fill factor in the solar cells and reduced bulk electron transport. We discuss these results considering the effects of morphology on charge separation.

[a] A.De Sion et al., Solar Energy Materials a. Solar Cells 95/12(2011)

CPP 6.9 Mon 17:30 Poster A

Charge transport investigation in electrochemical environment — •Zhiwei Yi[2], Bastian Kopp[2], Dirk Mayer[1], Andreas Offenhäusser[1], and Elke Scheer[2] — [1]Research Center Jülich, 52425 Jülich, Germany. — [2]Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Here, an electrochemical mechanical break junction setup is introduced, which combines electrodeposition techniques and mechanical breaking techniques. Using such setup, the charge transport through electrostatically assembled molecular junctions of Au/cysteamine/1,1-ferrocene dicarboxylic acid (FDA)/ cysteamine/Au was measured in liquid. The conductance across those single-molecule junctions (0.34 x 10^{-4} G_0) is one order of magnitude smaller than the conductance of covalently linked ferrocene molecular junctions (3.4 x 10^{-4} G_0), which indicates that the electrostatic coupling is strong enough to form an electron transport pathway, but the electron transfer rate across electrostatic interfaces is lower than across the covalent bonds. Molecular monolayers assembled on Au surface and Au/molecule/Au junctions are often used to investigate the influence of light on the electron transport across molecules. However, the influence of light on the charge transport at the liquid/metal interface has not been investigated yet. Here, using an indium tin oxide (ITO) electrode with gold nanoparticles on top as the working electrode, light induced signals were observed when performing cyclic voltammetry. We discuss voltage and wave-length dependence of the light-induced signals and first results obtained for photochromic molecules assembled with this technique.

CPP 6.10 Mon 17:30 Poster A

Time resolved microwave conductivity (TRMC) and transient absoption (TAS) measurements reveal charge carrier dynamics in organic semiconductors — •Andreas Fritze[1], Andreas Sperlich[1], Carsten Deibel[1], Tom J. Savenije[3], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, D-97074 Würzburg — [3]Department of Chemical Engineering, Delft University of Technology, NL-2628 BL Delft, The Netherlands

Understanding of the light induced charge carrier dynamics in self arranged organic semiconductors is essential to improve material properties and processing parameters and, at long sight, device performance. We performed combined TRMC and TAS measurements on organic semiconductors to gain direct access to the microscopic transport properties and charge carrier densities, respectively comparing both data yields us a complete picture about the generation, transport and recombination of charges on a microscopic length-scale. After laser pulse excitation TRMC and TAS signal decay in the blend of PCPDTBT:PCBM with varying PCBM content have been observed at different temperatures. This polymer:fullerene blend is a promising candidate for new high efficiency organic photovoltaic devices. We discuss the influence of morphology on light induced charge carrier density, recombination and mobility on a microscopic scale.

CPP 6.11 Mon 17:30 Poster A

Influence of PEDOT:PSS on the Morphology of P3HT:PCBM:PSS Solar Cells — •Ben Stafford, Klaus Wagenbauer, Eva M. Herzig, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

In organic photovoltaics the binary system poly(3-hexylthiophene) (P3HT) and phenyl C61-butyric acid methylester (PCBM) is well known for the active layer. By adding a third component, in our case polystyrenesulfonate (PSS), the performance of a solar cell can be improved. [1] PSS has no conductive or absorbing properties, consequently it must influence the morphology of the ternary system as compared with the two component system. Indeed, we have observed an ordering effect on P3HT when adding PSS to the binary blend. Of great interest is the interface between PEDOT:PSS and the active layer and its influence on the P3HT morphology. To optimise device performance different layer thicknesses of the PEDOT:PSS blocking layer are examined via electrical characterization.

[1] Kim et al., Solar Energy Materials and Solar Cells, 92:1188 (2008)

CPP 6.12 Mon 17:30 Poster A

Simulations of charge transport in lamellar PBTTT — •Alexander Malafeev[1,3], Eunkyung Cho[2], Chad M. Risko[2], Jean-Luc Bredas[2], Victor Ivanov[3], and Denis Andrienko[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, USA — [3]Physics Department, Moscow State University, Moscow, Russia

The force-field of poly(2,5-bis(3-alkylthiophen-2-yl)thieno[3,2-b]thiophenes) (PBTTT), a compound with a charge carrier mobility of up to 1 cm^2/Vs, is parametrized using first-principles calculations. Subsequently, molecular dynamics simulations of a lamellar molecular arrangement are performed and the charge carrier mobility is determined by solving rate equations[1] in large-scale morphologies of

PBTTT. We find that the unit cell parameters, as well as charge carrier mobilites, are in a good agreement with experimental data.

[1] V. Rühle, A. Lukyanov, F. May, M. Schrader, T. Vehoff, J. Kirkpatrick, B. Baumeier, D. Andrienko, J. Chem. Theory Comput., 7, 3335 (2011)

CPP 6.13 Mon 17:30 Poster A

Subsurface Mapping of Amorphous Surface Layers on different types of P3HT

— •M. Zerson[1], E.-C. Spitzner[1], C. Riesch[1], R. Lohwasser[2], M. Thelakkat[2], A. Sperlich[3], H. Kraus[3], V. Dyakonov[3], and R. Magerle[1] — [1]Technische Universität Chemnitz, Chemnitz, Germany — [2]Universität Bayreuth, Bayreuth, Germany — [3]Julius-Maximilians-University of Würzburg, Würzburg, Germany

We study the surface structure of different types of poly(3-hexylthiophene) (P3HT) using depth-resolved amplitude modulation atomic force microscopy. From a map of amplitude-phase-distance (APD) curves, the tip indentation into the soft (compliant) amorphous surface layer is measured. This spatial information serves as depth coordinate for reconstructing high resolution cross sections and 3D depth profiles of the top 10 nm of the specimen. Furthermore, the shape of the unperturbed (true) surface and the thickness of the amorphous top layer are can be determined. With this depth profiling technique we discovered that the entire surface of different types of (P3HT) is covered by an amorphous layer of P3HT. We determine the amorphous layer thickness of commercial P3HT with a wide range of molecular weight (PDI 1.97), purified commercial P3HT (PDI 1.59) and of a well-defined type of P3HT with a low polydispersity index (1.19). Its thickness is between 4 and 10 nm, depending on the type of material, sample preparation conditions and annealing. We discuss the possible impact of these amorphous surface layers on the electronic properties of the surfaces and the performance of thin-film electronic devices using these polymers.

CPP 6.14 Mon 17:30 Poster A

Tuning of Crystal Orientation in Conducting Polymer Blends

— •Eva M. Herzig[1], Klaus Wagenbauer[1], Volker Körstgens[1], Weijia Wang[1], Yuan Yao[1], Adeline Buffet[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[2] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]HASYLAB at DESY, 22603 Hamburg, Germany

Surface sensitive x-ray diffraction is a powerful method to investigate molecular orientation in thin conducting polymer films [1]. In organic electronics successful charge transport depends strongly on the structural arrangement of the organic components because charge transport is anisotropic in such materials. Therefore control over crystallization and crystal orientation is highly desirable to improve device performance.

Using grazing incidence wide angle x-ray scattering we are able to show that the addition of an amorphous, electrolytic polymer results in an increased molecular ordering in standard organic photovoltaic films. This ordering is examined with respect to different parameters like temperature and substrate surface thereby showing ways of deliberately influencing the polymer crystal orientation.

[1] J. Perlich, J. Rubeck, S. Botta, R. Gehrke, S. V. Roth, M. A. Ruderer, S. M. Prams, M. Rawolle, Q. Zhong, V. Körstgens, and P. Müller-Buschbaum, Rev. Sci. Instrum. 81, 105105 (2010)

CPP 6.15 Mon 17:30 Poster A

Increase in performance of polymer based field effect transistors with dielectric nanoparticles

— •Ali Veysel TUNC[1], Jürgen Parisi[1], and Elizabeth von Hauff[2] — [1]University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory (EHF) Carl-von-Ossietzky Str.9-11, 26129 Oldenburg, Germany — [2]Institute of Physics, University of Freiburg, Germany

We have investigated the effect of nanomorphologic manipulation by SiO2 nanoparticles and PCBM [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) in poly [2-methoxy,5-(3',7'-dimethyl-octyloxy)]-p-phenylene vinylene (MDMO-PPV) based field effect transistors. PCBM has already been observed to improve hole mobility when added to the polymer. The explanation of this improvement with PCBM is still controversial in the literature. We investigate the effect of conducting and insulating nanomaterials (SiO2 and PCBM) on the transport properties of PPV based field effect transistors. Scanning electron microscopy (SEM) is used to image the morphologies of the blends. We observe that both PCBM and SiO2 nanoparticles lead to an increase in the hole current and effect mobility, and additionally reduce the contact resistance and the threshold voltage. We discuss these improvements in terms of improved chain ordering and conformation. To confirm this, we additionally investigate the influence of SiO2 nanoparticles in blends prepared with PPVs of varying molecular weight. We demonstrate that using SiO2 nanoparticles then can be a simple and cost effective method to improve the performance in polymer based OFETs.

CPP 6.16 Mon 17:30 Poster A

Host-Guest Complexes of β-Cyclodextrin-Substituted Silicon (IV) Phthalocyanines and a Tetrasulfonated Porphyrin: MD Simulations and Estimates on Electron Transfer

— •Julie Krainau[1], Jörg Megow[1], Alexander Kulesza[2], and Volkhard May[1] — [1]Institut für Physik, Humboldt Universität zu Berlin, Germany — [2]Institut für Physik, Freie Universität zu Berlin, Germany

The development of artificial photosynthesis requires an assembly of molecules that can mimic light harvesting and charge separation. Two host-guest complexes are formed between a tetrasulfonated porphyrin and several silicon (IV) phthalocyanines. The latter are substituted axially with two permethylated β-cyclodextrin units via different spacers. For these compounds it had been shown that they satisfy the needed requirements by exhibiting photoinduced fluorescence resonance energy transfer and charge transfer .The experimental measurements led to the hypothesis that the host-guest complex with the longest spacer has two conformations: One folded conformation in which the spacer is bended in such a way that the donor-acceptor distance is decreased and one conformation in which the donor and the acceptor are not close to each other [1]. In order to analyse this hypothesis, room-temperature MD simulations, using water as solvent, have been conducted that proved the made assumption. Furthermore, the trajectory gained by MD simulations was used to estimate the charge transfer rate in its dependence on the conformation.

[1] Ermilov et al., Phys. Chem. Chem. Phys., DOI: 10.1039/c1cp21930h

CPP 6.17 Mon 17:30 Poster A

Role of Structural Order on Ultrafast Free Charge Generation in Polythiophene/Si Photovoltaics

— •Christina Scharsich[1], Daniel Herrmann[2], Sabrina Niesar[3], Martin Stutzmann[3], Eberhard Riedle[2], and Anna Köhler[1] — [1]Universität Bayreuth — [2]Ludwig-Maximilians-Universität München — [3]Technische Universität München

In hybrid and organic solar cells, the precise process for the generation of free charge carriers is still not fully understood. This is partially due to the ultrafast time scale of a few-10 fs on which charge transfer between e-donor and acceptor takes place. Here, we use a novel broadband ultrafast transient absorption spectroscopy with a time resolution of 40 fs to probe charge generation and recombination in thin films of poly(3-hexylthiophene)/silicon (P3HT/Si). The fundamental photophysical processes accompanying charge generation depend strongly on morphology of the heterojunction. For this reason, we study the role of structural order on the ultrafast charge generation by applying regioregular (rr) and regiorandom (rra) P3HT as electron donor material. [1,2] We show that singlet excitons dissociate to subsequently form polarons within 140 fs. Aggregated rrP3HT/Si films show recombination of non-geminate pairs. In comparison, geminate recombination appears to be the dominant loss mechanism for rraP3HT/Si films. Therefore, we find that polymer structural order is the key criterion for free charge generation in hybrid P3HT/Si solar cells.

[1] D. Herrmann et al. J. Am. Chem. Soc. 2011, 133, 18220-18233
[2] C. Scharsich et al. J. Polym. Sci., Part B: Polym. Phys. - in press

CPP 6.18 Mon 17:30 Poster A

Electronic trap states in organic polymer-fullerene solar cells

— •Julia Rauh[1], Stefan Neugebauer[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, D-97074 Würzburg

Trap states can have a significant influence on the performance of organic solar cells, as they lower the mobility, disturb the internal field distribution and affect the recombination dynamics. We investigated the trap states in the polymer P3HT as well as in fullerene derivatives commonly used as electron acceptors in organic bulk-heterojunction solar cells, namely $PC_{61}BM$, $PC_{71}BM$ and $bisPC_{61}BM$, by thermally stimulated current measurements. Hereby, broad trap distributions were revealed for all investigated materials. In addition to the pure materials also polymer-fullerene blends were studied, revealing even deeper trap states, which were not detected in the single materials, with the amount of these deeper traps depending on the preparation conditions of the solar cells. The investigations are complemented by current-based deep level transient spectroscopy yielding additional information about the emission rates of the traps, which is of fundamental importance to describe charge carrier dynamics, e.g. in transient experiments

CPP 6.19 Mon 17:30 Poster A

Structured Interfaces in Organic Photovoltaic Devices — •Claudia Maria Palumbiny[1], Robert Meier[1], Holger Christian Hesse[2], Ricky Dunbar[2], Lukas Schmidt-Mende[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik -Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]LMU München, Center for NanoScience (CeNS), Hybrid Nanostructures, Amalienstr.45, 80799 München, Germany

Precise control of the heterojunction morphology in thin films is one of the key issues for the improvement of organic photovoltaic (OPV) devices. Interdigitated interfaces of the organic material on the nanoscale provide ideal charge extraction pathways for separated charge carriers. Structured surfaces of the selective electrode on the lower microscale further allow to enhance the optical absorption of the thin film components due to light trapping. Two different ways of artificial structuring are under investigation: Using anodized aluminum oxide hard templates as stamps with controlled dimensions, nanostructured organic layers can be realized on ITO support. As shown recently, a sufficient replica of the template structure can be transferred into the organic compound[1]. Alternatively, master molds with nanoscale channels are used for the imprinting routine of the PEDOT:PSS layer. The shape of the imprinted structures is easily tunable by the concentration of an additional plasticizer. Depending on the structure dimensions the device efficiency of OPVs can be increased this way[2].

[1] Hesse et al., Nanotechnology, 22, 055303 (2011)

[2] Meier et al., DOI: 10.1039/C1JM13766B

CPP 6.20 Mon 17:30 Poster A

Influence of Nongeminate Recombination on the Field-Dependence of the Photocurrent in Organic Solar Cells — •Ian Howard, Ralf Mauer, and Frédéric Laquai — Max Planck Institute for Polymer Research, Mainz

The role of interfacial charge-transfer (CT) states in determining the bias dependence of the photocurrent in Organic Solar Cells is debated. Understanding the bias dependence of the photocurrent is necessary to optimize device fill factors, and therefore resolution of this debate is important. In this contribution we directly determine the field dependence of bimolecular recombination at the charge densities relevant to photovoltaic devices using a novel optical pump electrical probe experiment that enables the ultra fast time resolution of optical spectroscopy to be combined with high signal to noise achievable in current measurements.[1] We relate these results to temperature dependent transient absorption (pump-probe) spectroscopy over the entire relevant timescale from femtoseconds to milliseconds [2] We conclude that in the benchmark polythiophene:methanofullerene system nongeminate recombination plays a dominant role in determining the bias dependence of the photocurrent.

[1] R. Mauer, I.A. Howard, F. Laquai, J. Phys. Chem. Lett. 2011, 2 (14), 1736-1741.

[2] R. Mauer, I.A. Howard, F. Laquai, J. Phys. Chem. Lett. 2010, 1 (24), 3500-3505.

CPP 6.21 Mon 17:30 Poster A

Immobilization of quantum dots via conjugated SAMs and their application as a light-controlled sensor for the detection of hydrogen peroxide — •Waqas Khalid[1], Mira El Helou[1], Tobias Murböck[1], Zhao Yue[1], Jose-Maria Montenegro[1], Kirsten Schubert[2], Gero Göbel[2], Fred Lisdat[2], Gregor Witte[1], and Wolfgang Parak[1] — [1]Fachbereich Physik and WZMW, Philipps-Universität Marburg, Marburg, Germany — [2]Biosystems Technology, Technical University of Applied Sciences Wildau, Germany

A light-addressable gold electrode modified with CdS and FePt or with CdS@FePt nanoparticles (NPs) via an interfacial dithiol layer is presented. High-resolution synchrotron-based XPS measurements reveal that trans-stilbenedithiol (StDT) provides high quality self-assembled monolayers compared to benzenedithiol, biphenyldithiol (capped, uncapped) and capped StDT, in case they are formed at elevated temperatures. This alternative preparation evokes a discernible enhancement of lateral dithiol packing. The CdS NPs well immobilized on the dithiol layer allow for current generation under illumination and appropriate polarization. High quality of SAMs and the enhanced conductivity of their fully conjugated backbones impair a refinement in photocurrents and device performance by an order of magnitude. Moreover, FePt NPs serve as catalytic sites for the reduction of hydrogen peroxide to water. Advantageously, both NP properties can be combined by the use of hybrid NPs fixed on the electrode by means of the optimized StDT layer. This allows a light controlled analysis of different peroxide concentrations.[1] [1] W. Khalid et al. ACS Nano, 2011 (in print).

CPP 6.22 Mon 17:30 Poster A

Determination of the mobility and lifetime of charge carriers in organic solar cells under operating conditions — •Andreas Baumann[1], Jens Lorrmann[2], Daniel Rauh[1], Carsten Deibel[2], and Vladimir Dyakonov[1,2] — [1]Bavarian Center for Applied Energy Research (ZAE Bayern), Am Hubland, D-97074 Würzburg, Germany — [2]Experimental Physics VI, Physical Institute, Julius Maximilian University of Würzburg, Am Hubland, D-97074 Würzburg

The field of organic photovoltaics (OPV) is rapidly raising the last years with power conversion efficiency values exceeding 7%. For a better understanding of the performance and especially the limitations of these solar cells, it is, however, still essential to study the fundamental processes like the transport and the recombination dynamics of photogenerated charge carriers. A prominent experimental technique, which is more and more applied in the field of OPV, is the charge extraction technique CELIV studying both the mobility and lifetime of light induced charge carriers, simultaneously. However, there are several drawbacks, such as charge carrier injection causing large RC or inhomogeneous charge carrier profiles (non-steady-state conditions) resulted by the laser flash, which prevent a direct correlation to the solar cell working conditions. With our newly developed charge extraction technique OTRACE, it is now feasible to get new insights into the transport and the recombination dynamics in organic BHJ solar cells under operating conditions. Results are shown for the highly efficient solar cells of PTB7 and PCDTBT blended with [70]PCBM, whereas the I-V characteristics are correlated to the mobility and lifetime.

CPP 6.23 Mon 17:30 Poster A

Increasing the performance of vacuum-processed organic light-emitting pin diodes by inserting an solution-processed hole-transport layer — •Thorsten Umbach, Stefan Schneider, Heike Klesper, and Klaus Meerholz — Universität zu Köln, Department Chemie, Luxemburgerstr. 116, 50939 Köln, Germany

High ohmic losses and a poor charge injection are the main obstacles on the way to stable organic light emitting diodes (OLED's) with high-power efficiencies and low driving voltages. A promising technique to get rid of these drawbacks is a molecular doping of charge transport layers. Throughout the last decade this has been successfully applied in vacuum processed devices leading to pin OLED architecture with internal efficiencies approaching unity.

However, major improvements in the field of OLED technology can be made by improving the light out-coupling. In conventional device architectures around 80% of the generated light is lost within the layers due to total internal reflection, wave guiding, and absorption.

By inserting an additional nanoporous hole-transport layer (HTL) into an OLED system we gain a strongly enhanced light output. The external quantum efficiency is increased up to 20%. This enhancement is due to a lower film density and the resulting lower refractive index of the HTL.

Here, we demonstrate the combination of both techniques. By optimizing the light out-coupling-properties by the HTL and the electronic structure by doping, the resulting hybrid devices have great potential to overcome most of the drawbacks OLED devices still suffer from.

CPP 6.24 Mon 17:30 Poster A

Towards Highly Efficient Vacuum-processed Merocyanine Tandem Solar Cells — •Vera Steinmann[1], Nils Kronenberg[1], Hannah Bürckstümmer[2], Dirk Hertel[1], Martin Lenze[1], Steven Graf[1], Frank Würthner[2], and Klaus Meerholz[1] — [1]Department für Chemie, Universität Köln, Luxemburger Straße 116, 50939 Köln (Germany) — [2]Institut für Organische Chemie and Röntgen Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, 97074 Würzburg (Germany)

In the last decade, high demand for low-cost, renewable energy spurred strong developments in the research of organic photovoltaics (OPV).

To date, the highest power conversion efficiency (PCE) of 8.4% is reported for polymer solar cells. However, small molecules (SM) have recently gained increased interest, reaching PCEs around 6%. Admittedly, most efficient SM solar cells still require rather sophisticated multilayer device configurations. In the past, we successfully introduced merocyanine (MC) dyes in vacuum-processed (VAC) single solar cells with PCEs up to 4.9%. Further device optimization led to high PCEs beyond 6%, while maintaining a simple device setup. Impressive performances motivated the implementation of MCs in VAC tandem cells. We present a "proof of concept" MC tandem cell, consisting of two identical subcells. A high PCE of 4.7% is obtained, closely approaching the comparable single cell PCE of 5.0%. The optimized open-circuit voltage is as large as 2.1 V. Moreover, we introduce a novel tandem cell configuration, combining a planar- and bulk heterojunction. First MC tandem cells with different subcells are already highly promising.

CPP 6.25 Mon 17:30 Poster A

Structure and properties of reduced graphene oxide — •Michael Enzelberger[1], Siegfried Eigler[2], Philipp Hofmann[1], Christoph Dotzer[2], Andreas Hirsch[2], and Paul Müller[1] — [1]Department of Physics and Interdisciplinary Center of Molecular Materials, Universität Erlangen-Nürnberg, Germany — [2]Department of Chemistry and Pharmacy, Universität Erlangen-Nürnberg and Institute of Advanced Materials and Processes (ZMP), Germany

Reducing graphene oxide is an economic method for the large scale production of graphene. However, the reduction process causes a large number of defects. During thermal annealing of graphene oxide, CO_2 becomes mobile at around 50°C and a CO_2 intercalated compound is formed. This intermediate decomposes by the release of water and CO_2 at around 150°C as shown by thermogravimetric analysis and mass spectroscopy. Single flakes as well as sheets of flakes of the reduced graphene oxide were investigated. We characterize the quality of the samples by combining Raman spectroscopy and Hall mobility measurements. For high quality samples we find a Raman D/G ratio of 3 and Hall mobilities exceeding 10 Vs/cm^2.

CPP 6.26 Mon 17:30 Poster A

Modelling charge carrier dynamics in disordered semiconducting materials — •Jens Lorrmann[1], Julien Gorenflot[1], Vladimir Dyakonov[1,2], and Carsten Deibel[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — [2]Bavarian Center for Applied Energy Research e.V. (ZAE Bayern e.V.), Würzburg

Organic semiconductors are promising candidates for low cost electronic applications, i.e. organic solar cells or organic light emitting diodes. Their performance is now approaching market maturity. But still there is little known about the impact of energetic and spatial disorder present in these materials, on the charge carrier dynamics and thus on the performance. To gain further insight, we developed a time dependent multiple trapping and release model to track the fate of electrons and holes hopping in a gaussian or exponential density of sates (DOS). The tail states of the DOS act as trap-states, where as the charge carriers move freely above the transport energy with a temperature dependent mobility. We show how disorder influence thermalization, non-geminate recombination and transport. For instance the recombination rate strongly increases with increasing energetic disorder or decreasing temperature, which reproduces the experimentally observed deviations from the Langevin theory [1]. Furthermore, the model is capable to describe temperature dependent transient absorption measurements on poly(3-hexyl thiophene-2,5-diyl) (P3HT) blended with [6,6]-phenyl-C_{61} butyric acid methyl ester (PCBM).

[1] P. Langevin, Ann. Chim. Phys. 28, 433, 1903.

CPP 6.27 Mon 17:30 Poster A

Influence of Polarization on the Energy Landscape for Charge Transport in Organic Electronic Materials — •Falk May[1], Björn Baumeier[1], Denis Andrienko[1], and Christian Lennartz[2] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]BASF SE, GVC/E - B009, Ludwigshafen, Germany

Design of organic semiconductors for particular applications requires knowledge of the distribution of energy levels participating in charge transport. These levels are often approximated by EA/IP of single molecules in vacuum, while effects of the environment (broadening, shifts) are taken into account phenomenologically, using simple dielectric cavity or lattice models. Using a representative host-guest system of the active layer of an organic light emitting diode, we show that these approximations can be incompatible with the microscopic evaluation of site energy disorder in realistic morphologies. In a particular case of electron transport, microscopic polarization effects do not reduce the energetic disorder arising from static Coulomb interactions, in contradiction to the predictions of lattice models. Inclusion of polarization effects also leads to a relative shift of the guest and host distributions, which again cannot be rationalized within mesoscopic descriptions. Both effects lead to a strong overlap of site energy distributions and hence affect electron transport dynamics and the current distribution in the host-guest mixture.

CPP 6.28 Mon 17:30 Poster A

Controlled polymerization of electron-deficient monomers: controlled preparation of n-type semiconducting polymers for organic electronics — •Anton Kiriy and Volodymyr Senkockyy — Leibniz Institut für Polymerforschung Dresden

Electron-conducting(n-type) main-chain pi-conjugated polymers are commonly prepared via well-established step-growth polycondensation protocols which enable limited control over polymerization. Chain-growth catalyst-transfer polycondensations were recently developed for controlled preparation of only hole-conducting (p-type) semiconducting polymers and block copolymers. In this contribution we present a new synthetic protocols that allows preparation of well-defined n-type semiconducting polymers. Specifically, we report on controlled polymerization of naphtalene-diimide based monomer resulting into corresponding n-type conjugated polymer (PNDIT2) with controlled molecular weight, relatively narrow polydispersities, and specific end-functions. Electron mobility of this polymer will be also presented (Senkovskyy, Kiriy, et al. J. Am. Chem. Soc. 2011, ASAP, ja-2011-08710x).

CPP 6.29 Mon 17:30 Poster A

Built-in potential and validity of Mott-Schottky analysis in organic bulk heterojunction solar cells — •Markus Mingebach[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, D-97074 Würzburg

The built-in potential is an important key parameter of organic bulk heterojunction (BHJ) solar cells since it determines the internal electric field profile in the device but also gives an estimate for the open circuit voltage and hence the solar cell efficiency. The correct determination of the built-in potential is a nontrivial task, since zero field inside the BHJ device is not easy to achieve. We investigated poly(3-hexylthiophene-2,5-diyl):[6,6]-phenyl-C61 butyric acid methyl ester BHJ solar cells by means of temperature dependent measurements of the open circuit voltage and compared the results with the Mott-Schottky analysis of capacitance-voltage characteristics, which is a well-established tool to determine the built-in potential in inorganic devices. By applying the Mott-Schottky analysis to our solar cells we found considerably lower built-in voltages than expected from the difference of the electrode work functions. Moreover, a dependence of the built-in voltage, determined this way, on the active layer thickness of the devices was observed. We conclude that Mott-Schottky analysis seems not to be generally appropriate for the determination of the built-in potential in organic BHJ solar cells.

CPP 7: Poster: Biopolymers and Biomaterials (jointly with BP)

Time: Monday 17:30–19:30 Location: Poster A

CPP 7.1 Mon 17:30 Poster A

Conformation Changes of F-actin under Shear — •Inka Lauter[1], Donald Guu[2], Minne Paul Lettinga[2], Rudolf Merkel[1], and Margret Giesen[1] — [1]Institute of Complex Systems: Biomechanics (ICS-7), — [2]Institute of Complex Systems: Soft Condensed Matter (ICS-3); Forschungszentrum Jülich

Polymers have versatile physical characteristics. Besides stiff and flexible polymers, the class of semiflexible polymers is of high interest in rheology as well as in biophysics. In our work we focus on the collective properties of in vitro polymerized solutions of filamentous actin (F-actin). We present recent data on fluorescently labeled single actin filaments in a solution of unlabeled actin filaments under external shear force. The studies were performed by means of a multi-pinhole-confocal microscope and a counter rotating shear cell. We show that under shear, filaments align perpendicular to the velocity gradient. Furthermore we studied filament curvatures as a function of actin concentration. The curvature distribution exhibits an exponential tail and the probability for high filament curvatures increases with actin concentration. The distribution of filament lengths, however, is unaffected even under high shear rates. This result is in contrast to classic rheometer data, which predict filament rupture at a certain strain level.

CPP 7.2 Mon 17:30 Poster A

Diffusion and Adsorption of Proteins in Nanoscaled Environments — •Sebastian Mörz[1], Dagmar Auerbach[2], Gregor Jung[2], and Patrick Huber[1,3] — [1]Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Biophysical Chemistry, Saarland University, Saarbrücken, Germany — [3]Facultad de Física, Pontificia Universidad Católica de Chile, Santiago de Chile, Chile

During the recent years, some versatile developements in biochemistry have opened a wide field of applications. Examples are pore-suspending lipid bilayers or new means of drug delivery by encapsulation of biomolecules into mesoporous template materials. In nanometer scaled confinement, both the transport of biomolecules and their interaction with the porous environment are crucial to these applications, since the above mentioned systems employ artificial nanoporous matrices.

The aim of our research is to examine the diffusion and adsorption characteristics of proteins under such confinement in cylindrical nanochannels with special respect to the differences between the folded and the unfolded state of the proteins. Adsorption isotherms of folded and unfolded bovine heart cytochrome c in nanoporous silica have been measured at different pH-values, ranging from near-neutral pH to the isoelectric points of both the protein and the matrix. The diffusion of green fluorescent protein (GFP) in porous aluminum oxide was investigated using fluorescence correlation spectroscopy (FCS) for various pore diameters (25 to 75 nm) at pH 7 and at the isoelectric point of the membrane material (pH 9).

CPP 7.3 Mon 17:30 Poster A

Structural levels of organization in spider-silk - a combined mechanical and IR-spectroscopic study — •Markus Anton, Wilhelm Kossack, Roxana Ene, Christof Gutsche, and Friedrich Kremer — University of Leipzig, Institute of Experimental Physics I, Linnéstr. 5, 04103 Leipzig, Germany

Many efforts were undertaken to develop novel materials with promising mechanical qualities using spider silk as a pattern. Due to its unique mechanical properties, namely high tensile strength in combination with great elasticity, spider silk even surpass modern synthetic fibers like Kevlar [Kubik, *Angew. Chem. Int. Ed.* **41** (2002)].

Despite the successful synthesis of silk-like proteins, one is incapable to manufacture materials with similar properties on a large scale [Heim et al., *Angew. Chem. Int. Ed.* **48** (2009)], because of an incomplete understanding of spider silk's microscopic structure. Its mechanical properties are based on a refined architecture at the molecular and mesoscopic scale. Nanocrystals are interconnected by prestrained amorphous regions offering an internal pressure counterbalanced by the fiber's outer skin. By that structure, external stress is directly transferred to the nanocrystals resulting in a shift of the Alanin-specific absorption band [Papadopoulos et al., *Colloid. Pol. Sci.* **287** (2009), R. Ene et al, *Soft Matter* **5** (2009)].

To unravel this interplay between external and internal constrains a pressure- and temperature-dependent analysis of specific IR absorption bands by means of hydrostatic pressure provided by a diamond anvil cell was carried out.

CPP 7.4 Mon 17:30 Poster A

Frequency resolved depolarized light scattering studies of tRNA conformation in solution — •Christoph Angermann[1] and Thomas Hellweg[2] — [1]Universität Bayreuth, Physikalische Chemie 1 — [2]Universität Bielefeld, Physikalische und Biophysikalische Chemie

A custom built depolarized dynamic light scattering apparatus equipped with a confocal Fabry-Perot interferometer (FPI) with a free spectral range of 150 MHz was developed. The FPI is used to analyze the scattered light in the frequency domain. This is an important characteristic because the rotational motion of the particles modifies the depolarized component of the scattered light. Due to further development of this setup, it is easily possible to accumulate the noisy component efficiently leading to an enhancement of the signal to noise ratio. Combined with an iterative deconvolution method this apparatus can be used to analyze the rotational diffusion of tRNA from brewer's yeast in solution in a time range of 1 to 80 ns.

CPP 7.5 Mon 17:30 Poster A

(Visco-)Elasticity and thickness determination of polyelectrolyte multilayers by atomic force microscopy — •Johannes Hellwig, Cagri Üzüm, and Regine von Klitzing — Stranski-Laboratorium, Department of Chemistry, TU Berlin, Strasse des 17. Juni 124, D-10623 Berlin

Thin films of polyelectrolyte multilayers can be easily prepared by using the Layer-by-Layer technique. These films show different growth behaviour, e.g. linearly or non-linearly, and also different mechanical properties. Mechanical properties can be influenced by the hard substrate below the film. Therefore the film thickness has to be taken into consideration. The growth behaviour and film thickness of PEMs can be determined by different methods using an Atomic Force Microscope (AFM). A common method called *scratch method* and a newly presented method called *full-indentation* was used to determine the thickness of soft films with a double layer number of 12 * 96. It was shown that both methods agree well within the experimental errors. In addition the elastic modulus of the films was determined by using an Colloidal Probe AFM where a colloidal probe attached to the end of a cantilever was indented into the PEM film. The mechanical properties of the PEMs was calculated from the deflection of the cantilever with a Herzian based elasticity model. Latest research focus on the non-elastic behaviour of PEMs.

CPP 7.6 Mon 17:30 Poster A

Excitation energy transfer dynamics in the light-harvesting complex LH2 determined by a mixed quantum-classical approach — •Jörg Liebers[1], Carsten Olbrich[1,2], Mortaza Aghtar[1], Michael Schreiber[2], and Ulrich Kleinekathöfer[1] — [1]Jacobs University Bremen, Germany — [2]Chemnitz University of Technology, Germany

In photosynthesis the harvesting of sun light is done by light-harvesting antenna complexes containing chlorophyll and carotenoid molecules. Starting from the available crystal structure of the light-harvesting systems 2 (LH2) of a purple bacterium all-atom classical molecular-dynamics (MD) simulations were applied to obtain the motion of the nuclei due to thermal fluctuations [1]. These fluctuations provide the input for quantum chemical calculations to calculate the excitation energies of the Q_y states of the single bacteriochlorophyll (BChl) molecules and also the Coulomb couplings between them. Using these time series of excitation energies and couplings, the spectral density and time-dependent Hamiltonians for this system were constructed which allows for a quantum dynamical investigation of the excitation energy transfer processes in the LH2 complex [2]. Here we use ensemble averaged wave packet dynamics with a quantum correction for temperature effects to calculate excitation dynamics and optical properties.

[1] C. Olbrich, U. Kleinekathöfer, J. Phys. Chem. B 114, 12427 (2010).

[2] C. Olbrich, J. Liebers, U. Kleinekathöfer, phys. stat. sol. (b) 248, 393 (2011).

CPP 7.7 Mon 17:30 Poster A

Environmental effects on the exciton dynamics in the FMO light-harvesting complex — •Mortaza Aghtar[1], Carsten Olbrich[1], Jörg Liebers[1], Johan Strümpfer[2], Klaus Schulten[2], and Ulrich Kleinekathöfer[1] — [1]Jacobs University Bremen, Germany — [2]University of Illinois at Urbana-Champaign, USA

Long-lived quantum coherent transfer has been observed experimentally in Fenna-Mathews-Olson (FMO) light-haversting complex at a temperature of 77 K. The cause for these long-lived coherence is still unclear. Thermal effects of the environment have been studied widely as a possible answer not only at low but also at physiological temperatures. To contribute to this debate, we apply all-atom classical molecular-dynamics (MD) simulations to obtain thermal fluctuations of the environment. The MD calculations provide the input for quantum chemical calculations to obtain the vertical excitation energies of the single bacteriochlorophyll (BChl) molecules [1]. The distribution of energies and couplings are analyzed together with possible spatial correlations. Using excitation energies and couplings, we have constructed the spectral density and Hamiltonian of the FMO complex which allows for the investigation of exciton dynamics and environmental effects [1,2].

[1] C. Olbrich, Th. la Cour Jansen, J. Liebers, M. Aghtar, J. Strümpfer, K. Schulten, J. Knoester, and U. Kleinekathöfer, J. Phys. Chem. B 115, 8609 (2011).

[2] C. Olbrich, J. Strümpfer, K. Schulten, and U. Kleinekathöfer, J. Phys. Chem. Lett. 2, 1771 (2011).

CPP 7.8 Mon 17:30 Poster A

Selective decalcification: A method to determine the phosphate distribution within the cuticle of isopod by confocal Raman spectroscopy — •Christian Reisecker[1], Bastian Seidel[2], Andreas Ziegler[2], and Sabine Hild[1] — [1]Institute of Polymer Science, Johannes Kepler University, Altenbergerstrasse 69, 4040 Linz, Austria — [2]Central Facility for Electron Microscopy, University of Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

The mineralized exoskeleton (cuticle) of isopods, is an excellent model to study biological composite materials. In spite of the diversity of crustacean species they share a similar structural principle for their cuticle: An organic matrix composed of chitin-protein fibers associated with various amounts of crystalline and amorphous CaCO3 and Ca3PO4. Scanning confocal Raman microscopy (SCRM) is a useful tool to study the chemical composition isopod cuticle and to allocate the distribution of organic and inorganic components. Carbonate minerals can easily detected but phosphates are more difficult to assign because of their lower content and of their lower Raman intensity. In this study selective decalification at pH=7 is applied to determine the phosphate distribution within the cuticle of three different isopods, which mainly differ in their phosphate content. While the calcite layer appears to be unchanged after the procedure no ACC can be detected in the endocuticle. Performing Cluster analysis phosphates can be allocated within endocuticle. The influence of the phosphate content in the mechanical properties of the cuticle SFM nanodindentation experiments are performed.

CPP 7.9 Mon 17:30 Poster A

Using confocal spectroscopy to determine the Mg content and the crystalline orientation of calcite within the exocuticle of isopods — •Katja Huemer[1], Christian Reisecker[1], Martin Laher[1], Bastian Seidel[2], Andreas Zielger[2], and Sabine Hild[1] — [1]Institute of Polymer Science, Johannes Kepler University, Altenbergerstrasse 69, 4040 Linz, Austria — [2]Central Facility for Electron Microscopy, University of Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

The exceptional properties of biological composites, such as the exoskeleton of crustaceans, are based on a complex hierarchical architecture of inorganic and organic components. The mineralized exoskeleton formed by the cuticle of crustaceans is an excellent model to study biological composite materials. The cuticle consists of an organic matrix composed of chitin-protein fibers associated with various amounts of crystalline and amorphous calcium carbonate. Using scanning confocal Raman microscopy (SCRM) for isopods is was possible to show that mineral phases have a layered arrangement where calcite is restricted to the outer area of the cuticle forming the outer protective layer. The aim of this study is to investigate the influence of the Mg content and crystalline morphology in the mechanical properties of the exocuticle the tergites of three isopod species. Using SCRM for the different species the Mg content can be determined and different types of oriented growth of nanocrystalline calcite can be discriminated. SFM nanodindentation experiments are performed to show the influence of these parameters in the local mechanical properties.

CPP 7.10 Mon 17:30 Poster A

Phase transitions in Chitosan/DPPC membrane multilayer as a function of hydration — Zoraya E. Lopez Cabana, Carmen M. Gonzalez Henriquez, •Ulrich G. Volkmann, Patrick Huber, Marcelo Cisternas, Rosario Ortega, and Mauricio Sarabia — Surface Lab, Facultad de Fisica, Pontificia Universidad Catolica de Chile, Chile

The main goal of this investigation is the formation of porous membranes of chitosan, a natural polymer. The porous character favors the incorporation of humidity that affects the thermal behavior of the multilayer. The membranes have been formed by spin coating on silicon wafers at 2000/6000 rpm. The thickness of the membrane was studied with Very High Resolution Null Ellipsometry and their topography by Atomic Force Microscopy (AFM). On top of the chitosan membrane a precise concentration of DPPC was evaporated by Physical Vapor Deposition (PVD) and homogeneous DPPC films ($\sim$ 80 Åthickness) were obtained. The characterization of the phase transition temperature of the multilayer Chitosan/DPPC was realized by imaging ellipsometry and *in situ* AFM and Raman spectroscopy. These transitions are consistent with those found by Meyer *et al.* [1].

[1] Meyer, H. W.; Semmler, K.; Rettig, W.; Pohle, W.; Ulrich, A. S.; Grage, S.; Selle, C.; Quinn, P. J. *Chem. Phys. Lipids* **2000**, 105, 149-166.

C.M. G.H. acknowledges a scholarship from VRI Nr. 10/2010 (PUC). Work supported by FONDECYT project Nr. 1100882. Raman spectroscopy supported by FONDEF project Nr. D97F1001.

CPP 8: Poster: Nanoparticles and Composite Materials

Time: Monday 17:30–20:00 Location: Poster A

CPP 8.1 Mon 17:30 Poster A

Dielectric investigation of nanocomposites based on Polystyrene and Polyhedral Oligomeric Silesquioxanes — •Mohammad Mir Mohammad Sadeghi, Purv Purohit, Annabelle Bertin, Martin Böhning, and Andreas Schönhals — BAM Federal Institut for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany

Enhancement of polymer properties by use of different types of nanosized fillers has attracted a growing attention of scientists recently. Polymer based nanocomposites have shown improvement in properties as compared to conventional scaled composites because of the length scale of interaction between the nanofillers and the polymer matrixes. Efforts are made to fully understand the relationship between structure and properties of such polymer based nanocomposites. Nanocomposites of Polystyrene as matrix and MethacrylPOSS (MPOSS) as the nanofiller and crosslinker were synthesized. For preparation of the nanocomposites, different concentrations of MPOSS have been applied. In order to investigate the structure-property relationships of the nanocomposites, several methods such as dielectric relaxation spectroscopy, fourier transform infrared spectroscopy, differential scanning calorimetry, and thermal gravimetric analysis have been employed.

CPP 8.2 Mon 17:30 Poster A

Maghemite nanoparticles in thin block copolymer films — •Yuan Yao[1], Ezzeldin Metwalli[1], Volker Körstgens[1], Eva Herzig[1], Weijia Wang[1], Adeline Buffet[2], Stephan V. Roth[2], Matthias Opel[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]HASYLAB at DESY,

Notkestr. 85, 22603 Hamburg, Germany — [3]Walther-Meißner-Institut, Walther-Meissner-Str. 8, 85748 Garching, Germany

Maghemite nanoparticles embedded inside a polymer matrix mark a new class of hybrid materials which have attracted high interest. The control of the alignment of the maghemite nanoparticles within the polymer matrix is essential for producing well-aligned highly-oriented metal-polymer nanocomposites. The alignment of maghemite nanoparticles in poly(styrene-b-methyl methacrylate) diblock copolymer films is investigated. Two different sizes of maghemite nanoparticles are used: One is below and the other one above the critical particle size of the single magnetic domain. Films are prepared by solution casting within an external magnetic field. The morphology and inner nano-structure of the resulting hybrid films is studied as a function of the external magnetic field strength and for different concentrations of maghemite nanoparticles. The structure characterization of the films is based on optical microscopy, atomic force microscopy, and grazing incidence small-angle x-ray scattering. In addition, the magnetic properties are measured for different temperatures and compared with theoretical predictions.

CPP 8.3 Mon 17:30 Poster A

Structure-property relationship of Nanocomposites based on Polylactide and Carbon nanotubes — •Purv Purohit and Andreas Schönhals — BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany

The concept of biodegradable plastics is of considerable interest with respect to solid waste accumulation. Among numerous kinds of degradable polymers, polylactic acid sometimes called polylactide, an aliphatic polyester and biocompatible thermoplastic, is currently a most promising and popular material with the brightest development prospect and is considered as the *green* eco friendly material. So nanocomposites based on PLA and CNT can prove to be a promising class of material.

Nanocomposites with different concentrations of CNT in PLA were prepared via melt blending. The properties are studied using combination of various characterization techniques such as differential scanning calorimetry (DSC), small and wide angle X-ray scattering (SAXS & WAXS) and dielectric relaxation spectroscopy (DRS).

CPP 8.4 Mon 17:30 Poster A

Diffraction around a Single Heated Nanoparticle — •Markus Selmke, Marco Braun, and Frank Cichos — Universität Leipzig, Exp. Phys. I, molecular nanophotonics

Within the growing field of nano-sciences a fruitful new domain of metal nano-particles (NPs) has emerged: NPs of different shapes and composition have been used as markers, field-/ temperature-sources and sensors in many studies. Their unique and tunable absorptive properties are utilized in single particle photothermal (PT) detection which overcomes the scattering cross-section limitation of regular dark/wide-field and confocal microscopes. It is based on the (lock-in-)detected intensity-modulation of a probing laser beam caused by a particle-centered refractive index profile which is generated almost instantaneously through the absorption of a modulated heating laser. Thereby, even single molecules may be detected and a dispersion-like signature of the signal is obtained, which is what one would expect for a lens affecting the propagation of the gaussian probe beam. So far, no model exists which is able to describe the axial shape of the detected signal, nor does a quantitative theory for the signal magnitude exist at all. This gap, which so far separates this ultra-sensitive imaging technique from a quantitative tool, was bridged by the development of quantitative theories which are able to reproduce the full body of observed phenomena. One of them, the diffraction model presented here is shown to be particularly intuitive, quantitative and simple.

CPP 8.5 Mon 17:30 Poster A

Growth of silver nanowires within nanotubular J-aggregates — •Egon Steeg, Holm Kirmse, Jürgen P. Rabe, and Stefan Kirstein — Institut für Physik, Humboldt-Universität zu Berlin

It was demonstrated earlier that ultrathin but long Ag nanowires with a diameter less than 7 nanometers and a length exceeding micrometers can be fabricated by reduction of silver salt using uniform nanotubular J-aggregates of amphiphilic cyanine dyes as template [1]. Here we report on the growth mechanism of these Ag wires as revealed by transmission electron microscopy. The growth of the wires is photo-initiated by short illumination with blue light and is terminated at different time steps by removing Ag^+ ions upon adding NaCl to the solution. In this case the Ag^+ ions react with the Cl^- ions to form AgCl nanocrystals. At times shorter than 2 hours, small and well separated fragments of silver wires are found along the aggregates with a broad length distribution in the range of ten to hundred nanometers. At times later than 2 hours, homogeneous wires are found with lengths of microns filling almost the entire aggregates. By high-resolution TEM one finds microcrystalline domains with sizes up to 100 nm. These findings show that the growth of the wires starts independently at distinct nucleation centers and proceeds to fill the entire aggregate. This growth process must be supported by transport of Ag^+ ions through the tubular wall membrane.

[1] D.M. Eisele et al., J. Am. Chem. Soc. 132 (2010) 2104.

CPP 8.6 Mon 17:30 Poster A

Interfacial Properties of Grafted Nanoparticle Based Nanocomposites — •Mathias Meyer[1,2], Eike Hübner[3], Wim Pyckhout-Hintzen[1,2], Jürgen Allgaier[1,2], and Dieter Richter[1,2] — [1]Jülich Centre for Neutron Science, Forschungszentrum Jülich GmbH, Jülich, Germany — [2]Institute for Complex Systems, Forschungszentrum Jülich GmbH, Jülich, Germany — [3]Institut für Organische Chemie, Technische Universität Clausthal, Clausthal, Germany

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. They also reveal a core-shell-like structure of the non-grafted particles which has been neglected in literature so far. 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.

CPP 8.7 Mon 17:30 Poster A

Microscopic Characterization of Nanocomposites Featuring Attractive Polymer-Particle Interactions — •Thomas Glomann[1], Gerald Schneider[2], Wim Pyckhout-Hintzen[1], Jürgen Allgaier[1], and Dieter Richter[1] — [1]Jülich Centre for Neutron Science (JCNS-1) & Institute for Complex Systems (ICS-1), Forschungszentrum Jülich GmbH, D-52425 Jülich — [2]Forschungszentrum Jülich GmbH, JCNS am FRM II, Lichtenbergstr. 1, 85747 Garching

Attractive surface interactions between the particle and the polymer phase result in a layer of adsorbed chains on the particle surface which greatly influences e.g. the viscoelastic properties of the nanocomposite.

Poly(alkylene oxide)s (PAO)s mixed with bare silica nanoparticles are ideal model systems to gain microscopic insights on the role of surface interactions in nanocomposites. Strong attractive interactions are present between the OH-groups on the silica surface and the oxygen in the polymer backbone due to hydrogen bonding. Different sets of low and high molecular weight samples were prepared by solution blending of silica nanoparticles with appropriate mixtures of protonated and deuterated chains.

We present first results of our investigations of the microscopic chain structure and chain dynamics in the presence of adsorbing surfaces by means of using small-angle neutron scattering and neutron spin-echo spectroscopy.

CPP 8.8 Mon 17:30 Poster A

Continuous flow-through synthesis of prismatic silver nanoparticles in micro fluid segment sequences for possible SERS application — •Andrea Knauer[1], Andrea Csaki[2], Wolfgang Fitzsche[2], and Johann Michael Köhler[1,2] — [1]University of Technology Ilmenau, D-96893, Ilmenau, Germany — [2]Institute of Photonic Technology (IPHT) Jena, D- 07745, Jena, Germany

Non-spherical noble metal nanoparticles of gold and silver are of great interest due to their size- and shape-dependent plasmonic absorption in the long wavelength range. The spectral position of the in-plane dipole resonance wavelength can be tuned by the lateral length of the nanoparticles. It was expected that the homogeneity of nucleation and particle growth is influenced by the mixing speed due to the strong effect of reactant concentrations on the nucleation rate. Thus, the particle quality should improve, if high mixing rates under micro continuous-flow conditions and narrow residence time distributions are applied. The segmented flow technique was applied in order to combine a fast mixing by a segment-internal convection and a narrow residence time distribution. From the first synthesis step, homogeneous Ag seeds are obtained. In the second synthesis procedure, silver ions and a reducing agent are dosed into micro droplets containing Ag seeds in order to form silver nanoprisms, which display high size homogeneity. The presented technique can be adapted to synthesize colloidal solutions with tuneable particle sizes. Thus, the long-wavelength absorption can be shifted in a range between 520 and 1000 nm.

CPP 8.9 Mon 17:30 Poster A

Metal nanoparticle affected molecular emission: A density matrix approach — •Yuan Zhang[1,2], Yaroslav Zelinskyy[1], and Volkhard May[1] — [1]Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, D–12489 Berlin, Germany — [2]University of Science and Technology Beijing, XueYuan Road 30, 100083 Beijing, P. R. China

To compute the emission spectrum of a molecule metal nanoparticle complex a full quantum mechanical description of the system is presented. Based on a density matrix approach the computation accounts for intramolecular vibrational relaxation, nanoparticle plasmon damping, coupling to the photon field, and a non–perturbative consideration of the molecule nanoparticle interaction [1]. The latter is responsible for a remarkable plasmon induced decrease of the molecular radiative life–time. We investigate this life–time shorting in its effect on the time– and frequency resolved emission spectrum of the molecule nanoparticle complex. By including optical excitation of the system transient and steady–state spectra are presented.
[1] Y. Zelinskyy and V. May, Chem. Phys. Lett. **511**, 372 (2011).

CPP 8.10 Mon 17:30 Poster A

Time-resolved measurements on electron beam exposed Upconversion phosphors — •Manuela Reitzig[1], Thomas Härtling[1], Anton Mayer[2], and Jörg Opitz[1] — [1]Fraunhofer Institute for Nondestructive Testing IZFP, Dresden, Germany — [2]GigaTag GmbH, Oberpfaffenhofen, Germany

Since the development of infrared and Upconversion lasers and optical amplifiers, Upconversion materials have attracted significant attention. For several interesting applications trivalent rare-earth ions such as Er^{3+}, Tm^{3+}, Yb^{3+} and Y^{3+} were doped as luminescent centers in certain hosts such as oxysulfides and fluorides. Their unique optical properties depend on the host material and the dopant lanthanide ion and its concentration. Here we report on observation of alterations of the optical Up- and Downconversion properties due to electron beam treatment and discuss possible changes respective the crystalline and electronic structure of the material. The luminescence lifetime lasts for a few milliseconds and becomes sizably faster after electron beam treatment. We achieved to build up an optical set up we are able to obtain the decay time and spectrally resolved. With these observations we envisage a new application field for Upconversion phosphors, namely the optical, hence fast and contactless testing of e-beam irradiation. To this end rare-earth-based phosphors are placed as marker material inside or on a product packaging material. Upon electron irradiation the marker material changes its luminescent properties as a function of applied energy dose.

CPP 8.11 Mon 17:30 Poster A

Stabilizing Foams with Nanoparticles — •Adrian Carl and Regine von Klitzing — Stranski-Laboratorium, Institute of Chemistry, Berlin Institute of Technology, Strasse des 17. Juni 124, 10623 Berlin, Germany

In the recent years, it has been show by various groups that nanoparticles can be used to stabilize aqueous and oily foams [1]. The stabilization can be achieved without the use of surfactants. By appropriate tuning of the nanoparticle wetting properties, the adsorption of particles to the interface can be strongly favored. Due to the irreversible attachment of nanoparticles at the air/water interface, the surface elasticity and rheology of those foams is remarkably different from foams stabilized by surfactants. Various approaches can be used to hydrophobize particles. In addition, the process of foam formation has a strong impact on the resulting foam structure. An optimum in foamability of particle solutions is found for intermediate wettability.

Our work focuses on basic understanding of how the surface properties of modified silica nanoparticles influence their wetting behavior. Nanoparticles with varying degrees of functionalization and the resulting foams were characterized by scattering and microscopic techniques to gain insight into the governing principles of this comparatively young research field.

[1] A. Carl, R. von Klitzing, Angew. Chem., Int. Ed. 2011, 50, 11290-11292

CPP 8.12 Mon 17:30 Poster A

Photothermal spectroscopy studies of quantum dots in liquid crystals — •André Heber, Martin Pumpa, Markus Selmke, Marco Braun, Nicole Amecke, and Frank Cichos — Molecular Nanophotonics, University of Leipzig, Leipzig, Germany

Fluorophores have played an important role for single-molecule techniques but they suffer from bleaching which limits the observation time. Metallic nanoparticles can overcome this limitation. They constantly absorb light that is dissipated into the environment as heat. This temperature increase results in a change of the refractive index around the particle being detected by a probing laser beam. Usually gold nanoparticles are used as they have a large absorption cross section as compared to the 100-fold smaller one of quantum dots. We try to compensate this by observing quantum dots in a liquid crystal (5CB) slightly below the phase transition temperature from the nematic to the isotropic phase. A small heating of the quantum dot will cause the phase transition which results in a jump of the refractive index. Using this technique we are able to increase the photothermal signal by at least a factor of ten. We analyse the photothermal signal in liquid crystals and perform absorption spectroscopy on quantum dots as well as numerical calculations.

CPP 8.13 Mon 17:30 Poster A

Polymers in an aligned CNT array — •Marina Khaneft[1], Markus Domschke[1], Bernd Stühn[1], Rudolf Feile[1], Jörg Engstler[2], and Jörg Schneider[2] — [1]Experimentelle physik kondensierter materie TU Darmstadt — [2]Eduard Zintl-Institute für Anorganische und Physikalische Chemie TU Darmstadt

An aligned system of carbon nanotubes (CNTs) is obtained by noncatalytic chemical vapor deposition using templates of porous alumina (PAOX) with hexagonally ordered pores and removal of the alumina template. The 3D aligned CNTs array is mechanically stable, flexible and consists of freestanding, parallel aligned CNTs fixed by a carbon layer on one side. Obtained CNTs were used for preparation of CNT/polymer composites by melt infiltration of polystyrene (PS) into the free interstices of CNTs structure. Here we present an experimental study of polymer in aligned CNT array. Investigation is focused on the structure of the composites, polymer behaviour near the nanotubes. For quantitative analysis of the structure of the composites and control of the filling process small angle X-ray scattering was used. We applied differential scanning calorimetry to analyse a glass transition of the polymer inside the CNT array depending on the tube diameter and molecular weight of the polymer. Additionally, we applied Brillouin scattering and compare the sound propagation in different CNT/PS composites (vary diameter and molecular weight) with other nanoporous materials filled by polymer. The variation of the Brillouin spectra with the orientation of sample and scattering vector will be discussed.

CPP 8.14 Mon 17:30 Poster A

Investigation of wetting-dewetting transition of polymer grafted nanoparticles in polymer matrix — •Chang Jong Kim[1], Tinka Spehr[1], Bernd Stühn[1], Markus Mazurowski[2], Katrin Sondergeld[2], Roland Klein[2], and Matthias Rehahn[2] — [1]TU Darmstadt, Experimentelle Physik kondensierter Materie — [2]TU Darmstadt, Ernst-Berl-Institut für Technische und Makromolekulare Chemie

The dispersion of nanoparticles in a polymer matrix is generally improved by grafting polymers from the surface of the nanoparticles, when the grafted polymers are miscible with the surrounding matrix. For a given grafting density and molecular weight of grafted polymer the particle dispersion and wetting properties are known to sensitively depend on the ratio of the length of the surrounding polymer matrix to that of the grafted polymer chain. As the length of the matrix polymer chain exceeds that of the grafted polymer, chains of the polymer matrix are dewetted and particles aggregate. In our experiments polystyrene (PS, $M_n \sim 30$kDa) was grafted from spherical silica (SI) as well as deuterated polystyrene (d-PS) particles. These particles ($wt \sim 1\%$) were dispersed in d-PS matrices with various molecular weights and measured by small angle x-ray scattering (SAXS) and small angle neutron scattering (SANS). The particle dispersion and the change of the conformation (wetting-dewetting transition) of grafted PS chains are probed by analyzing SAXS and SANS scattering curves. First indication for dewetting mechanism were found for PS@d-PS particles when the molecular weight of PS matrix exceeded that of grafted PS.

CPP 8.15 Mon 17:30 Poster A

Polymerdynamics in Silicabased Nanocomposites with Attractive Interaction — •Barbara Gold[2], Gerald Schneider[2], Reiner Zorn[1], Juergen Allgaier[1], Wim Pyckhout-Hintzen[1], and Dieter Richter[1] — [1]Forschungszentrum Jülich GmbH Jülich Centre for Neutron Science (JCNS-1) & Institute of Complex Systems (ICS-1), Foschungszentrum Juelich GmbH, 52425 Jülich — [2]Jülich Centre for Neutron Science (JCNS), Forschungszentrum Jülich GmbH Outstation at FRM II, Lichtenbergstraße 1, 85747 Garching

The interactions between nanoparticles and polymerchains lead to a change in dynamics such as mechanical properties, dielectric relaxation and polymer dynamics.

Also the modification of the parameters within the sample preparation process (amount of solvent, time frame between adding nanoparticles and drying the sample) could modify the actual distribution of the particles as well as these dynamic quantities.

This poster shows the results of SAXS, broadband dielectric and linear rheology measurements concerning a PBO-Silica-System under the variation of particle concentration as well as sample preparation parameters named above.

CPP 8.16 Mon 17:30 Poster A

Blinking of single CdSe/ZnS nanoparticles on an Al covered silicon substrate — •Andreas Mölleken, Daniel Braam, Günther M. Prinz, Martin Geller, and Axel Lorke — Fakultät für Physik and CeNIDE, University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany

Semiconductor nanoparticles have attracted great interest as tunable light emitters. They can be easily fabricated without a solid state matrix and therefore placed into different environments and coupled to other nanostructures and metal surfaces. However, a drawback (and a phenomenon that is not yet understood in detail) remains: the blinking and spectral diffusion mechanism in the luminescence behaviour of single nanoparticles [1]. Previous studies have shown that the blinking behaviour is changed if the nanoparticles are close to a metal surface. In this study, we investigate the coupling between single nanoparticles and an Al metal surface. We fabricate a solution consisting of CdSe/ZnS core/shell nanoparticles dispersed in toluene with 1% PMMA and spin-coat this dispersion on top of an aluminium covered silicon substrate. For the measurements we use a μ-PL setup with two different excitation sources (405nm/532nm) in wide-field illumination. The setup enables us to study simultaneously many single nanoparticles and their luminescence behaviour. Our measurements show a blinking behaviour of the emission of single nanoparticles, which we can evaluate in terms of their characteristic on- and off-time statistics. Additionally we observe a slow blue shift in the emission energy over long time periods.

[1] Frantsuzov et al., Nature Phys. **4**, 519 (2008)

CPP 8.17 Mon 17:30 Poster A

DFT studies of clusters in external fields — •Manuel Matt, Marcus Beck, and Peter Nielaba — University of Konstanz, Department of Physics, 78457 Konstanz, Germany

Density functional theory (DFT) studies on the stability and structural properties of small clusters are performed. One point of interest is the arranging of diverse Si nano clusters. We use external electrostatic fields for ordering purposes of these clusters by polarization effects. Here we could stabilize a chain of up to five Si_7 clusters in a Car-Parrinello MD simulation with the CPMD package. We further investigate the $Al_{13}H$ cluster which has several isomers with different positions of the hydrogen atom. We analyze the effects of electrostatic and magnetic fields on these systems in order to explore the possibility to switch the isomers by external fields. For this we are using the OCTOPUS package. We found a switching between the two isomers of the neutral $Al_{13}H$ cluster at high magnetic fields.

CPP 8.18 Mon 17:30 Poster A

Separating interface from melt dynamics in a model system — •Christian Mark[1], Martin Brodeck[1], Wim Pyckhout-Hintzen[1], Jürgen Allgaier[1], Eike Hübner[2], and Dieter Richter[1] — [1]JCNS-1 & ICS-1, Forschungszentrum Jülich GmbH, Jülich, Germany — [2]Institut für Organische Chemie, TU Clausthal, Clausthal, Germany

Designing polymer-based materials with improved properties is an increasingly important field of polymer science. One particular area of interest within that field are the so-called polymer nanocomposites, which are made up of polymer and nanosized filler particles. It is our intent to connect the macroscopic properties of these composite materials to microscopic structure and dynamics.

The dynamics of these systems are, however, a quite difficult topic to study in microscopic detail. This is due to the generally large polydispersity of the nano-components as well as the fact that the measured dynamics are usually a mixture of both interface and melt dynamics. We were able to create grafted nano-sized silica particles (r = 7nm) with a large grafting density (0.7 per square nm, 5K PI), which should provide a sufficient "screen" for separating interface dynamics from melt dynamics. In addition, the grafted particles also allow us to study the dynamics of the grafted polymer chains themselves.

The method used to study the microscopic dynamics is inelastic neutron scattering (Neutron Backscattering and Neutron Spin Echo).

CPP 8.19 Mon 17:30 Poster A

Synthesis of Semiconductor Nanowires Based on Tubular J-Aggregates Template — •Yan Qiao, Frank Polzer, Holm Kirmse, Egon Steeg, Stefan Kirstein, and Jürgen P. Rabe — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin, Germany

Organic/inorganic hybrid nanomaterials, that combine the strengths of the individual materials while compensating for deficits, have recently attracted more and more attention. Quasi one-dimensional (1-D) nanomaterials, such as wires and tubes, have been intensively investigated owing to the beneficial influence of dimensionality on electronic and optical properties [1]. Based on former results on silver [2], this work focuses on the fabrication of quasi 1-D organic/inorganic hybrid nanostructures consisting of nanotubular J-aggregates self-assembled from amphiphilic cyanine dyes and filled with semiconductor nanowires such as ZnO. Owing to electrostatic interactions, zinc ions might adsorb at the outer and inner wall of the negatively charge surface of the tubular J-aggregates. Following the procedures of ammonia precipitation and subsequent heating to moderate temperatures, the transformation from zinc ions into ZnO within the hollow space of the tube with diameters less than 10 nanometers is supposed to be realized. The as-synthesized inorganic structures are identified by transmission electron microscopy and UV-Vis spectroscopy.

[1] Y. N. Xia et al., Adv. Mater. 2003, 15, 353.

[2] D. M. Eisele et al., J. Am. Chem. Soc. 2010, 132, 2104.

CPP 8.20 Mon 17:30 Poster A

Measuring the range of plasmonic interaction — Mareike Kiel[1], Madlen Klötze[1], •Steffen Mitzscherling[1], and Matias Bargheer[1,2] — [1]Institute of Physics and Astronomy, University of Potsdam — [2]Helmholtz Zentrum Berlin

When gold nanoparticles are covered with nanometric layers of transparent polyelectrolytes, the plasmon absorption spectrum A(λ) increases by a factor of approximately three and shifts to the red. These modifications of dissipative experimental observables stop when the covering layers become thicker than the particle diameter. The spectral modification of dispersive parameters like the reflection R, however, keeps changing with increasing cover layer thickness. The shift of the plasmon resonance caused by two interacting particle layers is studied as a function of the separating distance between the two layers. We discuss these observations in the context of an effective medium theory and conclude that it can only be applied for a layer thickness on the order of the particle diameter.

CPP 8.21 Mon 17:30 Poster A

New Perspectives of Twin-Focus Photothermal Correlation Spectroscopy — •Romy Schachoff, Markus Selmke, Marco Braun, and Frank Cichos — Universität Leipzig, Exp. Phys. I, MONA

Photothermal microscopy has been used successfully for the detection of non-fluorescent nano-objects such as gold nanoparticles, quantum dots or carbon nanotubes. It employs a local temperature field around a laser excited absorber inducing a local refractive index change which is detected by a second laser. A careful investigation of the mechanisms and the origin of the photothermal signal has shown that the photothermal detection volume is in general a twin-focus with two well separated axial detection regions that differ in their signal phase. With the help of this clear spatial separation we are able to measure low axial flow velocities on a short length scale by a cross correlation analysis. We have investigated the diffusion of gold nanoparticles in water by means of this so called Twin-PhoCS. Radiation pressure induced flow velocities are extracted and the detection limits for velocities and small displacements are explored with the help of small gold nanoparticles in the twin-focus.

CPP 8.22 Mon 17:30 Poster A

Motion and Fluorescence of Charged Single Quantum Dots in an Electric Field — •David Plotzki, Nicole Amecke, and Frank Cichos — Molecular Nanophotonics Group, University Leipzig

Semiconductor Quantum Dots exhibit several interesting optical properties, one of them being a characteristic photoluminescence intermittency (blinking) which is not yet fully understood. It is assumed to be closely linked to charges that influence the underlying relaxation processes.

We study the motion and intensity of CdSe/ZnS Quantum Dots dispersed in toluene and dodecane in the presence of an electric field (up to 200 V/cm). A wide-field microscope setup is used to capture and track the particles. From this, the relative intensities and drift velocities can be determined and conclusions about present charges can be drawn.

We are seeking to observe the exchange of charges at the electrodes by a change in the fluorescence state.

CPP 8.23 Mon 17:30 Poster A

Scanning transmission x-ray microscopy and quantitative analysis of thermoresponsive microgels — •Andreas Späth[1], Birgit Graf-Zeiler[1], Shivkumar Ghugare[2], Gaio Paradossi[2], and Rainer H. Fink[1] — [1]Friedrich-Alexander Universität Erlangen-Nürnberg, Physical Chemistry II, Erlangen, Germany — [2]Università di Roma Tor Vergata, Scienze e Tecnologie Chimiche, Rome, Italy

Microgels have attracted greater attention in a broad field of medical science. They unify features of macroscopic hydrogels like the connectivity and the responsivity to environmental changes with the colloidal characteristics of nano- or micro-sized systems. To gain deeper insight into the processes occurring during heating above the volume phase transition temperature, we investigate PVA/poly(methacrylate-co-N-isopropylacrylamide) based networks using scanning transmission X-ray microspectroscopy. The PolLux-STXM (SLS) combines local-spot chemical information (NEXAFS) and imaging with a resolution limit below 30 nm. Therefore we recheive new insight into the nanoscale properties of these materials and directly observe the shrinking behaviour of thermoresponsive microgels in aqueous solution in situ [1]. NEXAFS studies confirm the chemical stability of the particles above the volume phase transition temperature [2]. The qualitative analysis of the recheived transmittance profiles bases on the Lambert-Beer expression corrected by the finite width of the focused X-ray beam.

[1] Graf-Zeiler, B., et al., ChemPhysChem, 2011, DOI: 10.1002/cphc.201100370.

[2] Ghugare, S., et al., Macromolecules, 2011, 44 (11), 4470.

CPP 8.24 Mon 17:30 Poster A

Ellipsometry on GLAD samples: Applications and model calculation — •Johannes F. H. Risch[1], Matthias Schwartzkopf[1], Mottakin M. Abul Kashem[1], Gunthard Benecke[1,2], Adeline Buffet[1], Denise Erb[1], Berit Heidmann[1], Gerd Herzog[1], Volker Körstgens[3], Ezzeldin Metwalli[3], Roman Mannweiler[1], Jan Perlich[1], André Rothkirch[1], Kai Schlage[1], Peter Müller-Buschbaum[3], Ralf Röhlsberger[1], Rainer Gehrke[1], and Stephan V. Roth[1] — [1]DESY, Notkestr. 85, D-22607 Hamburg — [2]MPIKG, Dep. Biomat, Am Mühlenberg 1, D-14424 Potsdam-Golm — [3]TU München, Physik Department E13, James-Franck-Str. 1, D-85748 Garching

Polymers combined with metals have a wide field of application in technology and industry. For the installation of tunable optical properties in nanocomposites, glancing angle deposition (GLAD) [1] has been proven to be a reliable method due to the high acceptance of vacuum sputter deposition in industrial processes. We investigated glancing angle deposition of gold on top of a colloidal array (polystyrene nanospheres), which serves as nucleation points for gold clusters. Using Imaging ellipsometry, we investigated the change of optical properties caused by structural deposition of polystyrene-nanospheres and gold layers. On the basis of gold pins, being inclined with respect to the surface normal, on polystyrene spheres we obtain a change of the refraction indices and a varying apparent layer thickness as function of the orientation of the GLAD sample.

[1] Gonzalez-Garcia et al., ChemPhysChem 11, 2005 (2010)

CPP 8.25 Mon 17:30 Poster A

Humidity-tunable electronic conductivity of polyelectrolyte multilayers doped with Au-nanoparticles — Annika Ziegemeier, Cornelia Cramer, and •Monika Schönhoff — Institute of Physical Chemistry, Westfälische Wilhelms-Universität Münster, Corrensstr. 28/30, 48149 Münster, Germany

The dc conductivity of polyelectrolyte multilayers doped with gold nanoparticles (Au-nP) was investigated as a function of relative humidity. For this purpose, multilayers composed of poly(ethyleneimine) (PEI) or poly(allylamine hydrochloride) (PAH) and Au-nP (diameter about 20 nm) were built up using the layer-by-layer self assembly technique. Different polyelectrolytes and varying salt concentrations lead to differences in the total layer thickness and the Au-nP coverage, i.e. different interparticle distances. The dc conductivity of the doped systems is six orders of magnitude higher than that of ions in undoped multilayers, thus an electronic conductivity can be concluded. Electrons are transported via connected pathways of Au-nP, as concluded from the conductivity scaling inversly with the expected particle distance in different systems. With increasing relative humidity (RH) the dc conductivity decreases and reversibly increases again when RH is decreased. It is concluded that the swelling of the polyelectrolyte chains between adjacent particles leads to a loss of connectivity of the electronic pathways between single particles, driving the system closer to the percolation threshold, and resulting in a decrease of conductivity. In conclusion, the conductivity of polyelectrolyte multilayers doped with Au-nP can be reversibly tuned by varying the relative humidity.

CPP 8.26 Mon 17:30 Poster A

Studies on microgel-polymer blends — •Florian Schneider[1], Gerald Johannes Schneider[1], Andreea Balaceanu[2], Andrij Pich[2], Wim Pykhout-Hintzen[3], Jürgen Allgaier[3], and Dieter Richter[3] — [1]Jülich Centre for Neutron Science, 85747 Garching, Germany — [2]DWI an der RWTH Aachen e.V., 52056 Aachen, Germany — [3]Jülich Centre for Neutron Science & Institute for Complex Systems, Forschungszentrum Jülich GmbH, 52425 Jülich

Microgels are formed by crosslinking of single polymer chains. Possible characteristics of the resulting structures can include sensitivity to light, temperature and to chemical properties of the solvent. The response of the gel affect it's physical structure, for example changes in particle size or density. Up to now, studies mainly concentrate on microgels dissolved in water.

Combining the idea of filler particles to tune the properties of a polymer matrix with the concept of microgels, new and interesting composites can be imagined. Not only does the usage of soft, organic fillers result in lower compound weights, it also opens the possibility to influence the composites' properties by varying external parameters.

Our studies are based on custom poly(vinylcaprolactam) microgels. Their physical structure and it's dependency on the properties of the solvent as well as the possibility of dispersing them in a polymer matrix were resolved by different neutron scattering techniques. Moreover first results concerning their influence on the dynamics of a polymer matrix were obtained in rheology-experiments.

CPP 8.27 Mon 17:30 Poster A

Surface Charges on CdSe/ZnS Quantum Dots in Apolar Solvents — •Nicole Amecke and Frank Cichos — Molecular Nanophotonics Group, University of Leipzig

Despite intensive research, semiconductor quantum dots (QDs) show many peculiar fluorescence characterstics (blinking, flickering, spectral diffusion) that are not fully understood today. Many of those are expected to be strongly influenced by charges in the QD core or its close proximity. With a confocal microscope and an electrophoretic cell, charged QDs in solution can be detected and separated from neutral QDs while monitoring their fluorescence. Depending on solvent and electrode characteristics we find the percentage and polarity of detected fluorescent charges to differ, showing a manipulation of the charges at the electrode. This charging of QDs and their total percentage can also be detected by the current flowing through the device. Spectra and lifetimes from charged and neutral QDs are taken separately and compared. As only minor differences are found, the charge must be located at the surface not in the core.

CPP 8.28 Mon 17:30 Poster A

Polymer-Functionalized Carbon Structures: A Raman Spectroscopy View — •Evgeniya Sheremet, Raul D. Rodriguez, Thomas Ebert, Susanne Höhne, Stefan Spange, Ovidiu D. Gordan, and Dietrich R. T. Zahn — Chemnitz University of Technology, D-09107 Chemnitz, Germany

Raman spectroscopy is a powerful technique for structural studies of polymer-coated carbon structures. Here, we discuss the challenges of obtaining reliable Raman data and their interpretation using several model systems: phenolic resin on graphite flakes and poly(ethylhexylacrylate) with a pyrene headgroup, polyvinylamin, and polyacrylamide adsorbed on multi-wall carbon nanotubes (MWCNT). It is shown that such composites reveal clear G and D bands (around 1582 cm^{-1} and 1350 cm^{-1}, respectively) characteristic of carbon structures with sp^2 hybridization, and modifications induced by the polymer coating are discussed. From all polymers studied the largest degree of interaction with MWCNT was found for poly(ethylhexylacrylate) as deduced from an upward shift of the G peak mostly likely due to compressive forces induced by the polymer on the nanotube walls. However, organic materials, as well as carbon structures, can be strongly affected by laser irradiation. It was shown that phenolic resin is removed by UV excitation, what resulted in a decrease in its Raman signature. Pure MWCNT also demonstrate a decrease of D peak after laser irradiation. In this work a systematic analysis of D and G band shifts in Raman spectroscopy of polymer-carbon composites is presented.

CPP 8.29 Mon 17:30 Poster A

Particle Nanosomes with Tailored Silhouettes — Claudia Wagner[1], •Andrea Fortini[2], Eddie Hofmann[1], Thomas Lunkenbein[3], Matthias Schmidt[2], and Alexander Wittemann[1] — [1]Physikalische Chemie I, Universität Bayreuth, Universitaetsstr. 30, D- 95440 Bayreuth, Germany — [2]Theoretische Physik II, Universität Bayreuth, Universitaetsstr. 30, D-95440 Bayreuth, Germany. — [3]Anorganische Chemie I, Universität Bayreuth, Universitaetsstr. 30, D- 95440 Bayreuth, Germany.

We investigate the assembly of submicron capsules with walls that consist of a single layer of nanoscopic inorganic constituents. Nanoparticles and oppositely charged polymer colloids were joined at the surface of evaporating emulsion droplets. The heteroaggregates exhibited well-defined core-shell morphologies, with clusters of the polymer colloids as the core and a dense monolayer of nanoparticles as the shell. Subsequent removal of the polymer core led to capsules, which exhibited regular compartmentalized shapes. A high density of nanopores was obtained on objects with dimensions of less than half a micron. Regardless that the capsules consisted of a single layer of nanoparticles with few contacts keeping them together, they did not collapse or break apart. Monte Carlo computer simulations demonstrated that the nanoscopic constituents can be trapped into structurally arrested states.

CPP 8.30 Mon 17:30 Poster A

Preparation and Controlled Organization of Cubic-Shaped Gold Nanoparticles for the Generation of High-Harmonics — •Valerie Mondes[1], Sarah Metzke[1], Matthias Buchholz[1], Matthias Kling[2], Jürgen Plenge[1], Eckart Rühl[1], and Christina Graf[1] — [1]Freie Universität Berlin, Institut für Chemie und Biochemie, Physikalische und Theoretische Chemie, Takustr. 3, 14195 Berlin — [2]Max-Planck Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching

Strong plasmonic enhancement effects are expected from ordered patterns of anisotropic noble metal nanoparticles. Instead of using lithographically fabricated nanostructures, we prepare gold nanoparticles by methods of colloidal chemistry. For the preparation of cubically shaped gold nanoparticles we improved known literature procedures [1]. The conditions during the formation of the nanoparticles have been systematically varied in order to receive monodisperse gold nanocubes. It turned out that the exact composition of the shape-controlling surfactant cetyltrimethylammonium bromide (CTAB) plays a crucial role for the growth of the nanoparticles. Therefore, CTAB samples were purchased from different manufactures and their composition was analyzed regarding the presence of other halides, which are supposed to influence the particle growth. In addition, the influence of the temperature has been investigated. A self-organization method at liquid-liquid interfaces has been used to receive such ordered particle assemblies [2]. [1] P.N.Sisco, C.J.Murphy, J.Phys.Chem. A, 113, 3973 (2009). [2] Li, Huang, and Sun Angew. Chem. Int. Ed., 45, 2537 (2006).

CPP 8.31 Mon 17:30 Poster A

Photoluminescence quantum yield of near-infrared emissive nanoparticles — •Soheil Hatami[1], Christian Würth[1], Markus Grabolle[1], Susanne Leubner[2], Vladimir Lesnyak[2], Nikolai Gaponik[2], Alexander Eychmüller[2], and Ute Resch-Genger[1] — [1]BAM Federal Institute for Materials Research and Testing, Berlin, Germany — [2]Physical Chemistry/Electrochemistry , TU Dresden, Dresden, Germany

Semiconductor nanocrystals (quantum dots, QDs) are applied as fluorescent labels and active components in optical devices. QDs emitting in the near-infrared (NIR) and infrared (IR) region like CdTe, CdHgTe, and HgTe are of increasing importance, due to their high photoluminescence quantum yields (QY) compared to any other chromophore at wavelengths above 900 nm. Characterization of their performance requires reliable methods for the determination of QY under application-relevant conditions. For often performed relative optical measurements, standard dyes with precisely known QY are mandatory, with the lack of reliably assessed QY standards for the NIR and IR hampering the performance of such measurements. We established relative and absolute optical methods for the determination of QY of such QDs in this wavelength region. Therewith, we obtained the QY of these QDs from 1.) comparison of the integral emission of the QDs and standard dyes and 2.) absolute measurements of the ratio of emitted and absorbed photons using a calibrated and validated integrating sphere setup.

CPP 8.32 Mon 17:30 Poster A

Probing the electronic state of a single coronene molecule by the emission from proximate fluorophores — •Kathrin Schneider[1], Burkhard Fückel[1], Gerald Hinze[1], Klaus Müllen[2], and Thomas Basché[1] — [1]Institut für Physikalische Chemie, Johannes Gutenberg-Universität, 55099 Mainz — [2]Max-Planck-Institut für Polymerforschung, 55128 Mainz

Electronic transitions of the 2D-graphene type molecule hexabenzocoronene (HBC) have been measured at the single molecule level. The large intersystem crossing rate and long triplet state lifetime in the range of seconds are prohibitive for direct single molecule observation. By covalently coupling fluorescent acceptor molecules (perylenecarboximide, PMI) to HBC, efficient singlet energy transfer gives rise to strong PMI fluorescence. Confocal single molecule fluorescence microscopy with two excitation colours matching the HBC and PMI transition frequencies, respectively, was conducted. Single HBC-6PMI molecules were observed via the PMI emission. It was found that after selective excitation of the HBC the PMI emission is interrupted by dark intervals whose length of several seconds is in agreement with the triplet state lifetime of HBC. Accordingly, the presence/absence of PMI emission permits to read out the spin state of a single HBC molecule. Moreover, due to spectral overlap, the HBC triplet state acts as an energy acceptor for PMI in the excited singlet state, thus leading to efficient singlet-triplet annihilation (STA) during its lifetime. Hence, intersystem crossing into the HBC triplet state serves as a collective fluorescence switch for individual multichromophores.

CPP 8.33 Mon 17:30 Poster A

Investigation of interphases in polyethylenepropylene(PEP)-silsesquioxane-nanocomposites by positron annihilation lifetime spectroscopy — •Christian Ohrt[1], Tönjes Koschine[1], Stephan Harms[1], Klaus Rätzke[1], Franz Faupel[1], Gerald Schneider[2], Lutz Willner[2], and Dieter Richter[2] — [1]Materialwissenschaft-Materialverbunde , Universität Kiel, 24143 Kiel — [2]Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich

Free volume studies were performed in polymer-nanocomposites by positron annihilation lifetime spectroscopy (PALS) to explore the influence of the interphase nanoscale character of the filler particles and the nanoscale particle size on positron parameters. A weakly repulsive system was obtained by mixing of poly(ethylene-alt-propylene) (PEP) and silsesquioxane nanoparticles with varying concentration. DSC experiments showed a constant glass transition temperature Tg of the polymer and a phase transition of the filler at low temperature. PALS measurements showed a constant glass transition temperature Tg of the polymer, an increase of the free volume at the phase transition of the filler and a strong drop of the thermal expansion coefficient above Tg with increasing filler concentration. By changing the composition of the samples and applying a simple mixing rule for the lifetime spectra of the ortho-positronium, information about the existence of an interphase with properties different from the polymer matrix could be obtained.

CPP 8.34 Mon 17:30 Poster A

Evolution of lateral structures during the functional stack build-up of P3HT:PCBM based bulk heterojunction solar cells — •Shuai Guo[1], Matthias Ruderer[1], Christopher Birkenstock[1], Ezzeldin Metwalli[1], Monika Rawolle[1], Jan Perlich[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany

Solution-processable organic photovoltaics have shown great promise for providing an entirely new generation of ultralow-cost, lightweight, and flexible electronic devices, which would be an ideal alternative to replace the traditional expensive silicon-based semiconductors. Here, the most prominent material system 1,2-dichlorobenzene solution processed P3HT:PCBM bulk heterojunction (BHJ) solar cells, are prepared and investigated at different steps of the multi-layer stack build-up. The inner structural characteristics are probed with grazing incidence small angle X-ray scattering (GISAXS) and X-ray reflectivity. The surface morphology is detected with atomic force microscopy. Therefore, an in-depth knowledge of three-dimensional morphology of the polymer-based solar cell, starting from the cleaned ITO substrate up to the final post-treated solar cell, is generated. Three noticeable lateral structures, originating from the substrate, the active layer and the aluminum electrode, are detected with GISAXS. The correlation between nanostructure within the thin films and the solar cell efficiency are addressed.

CPP 8.35 Mon 17:30 Poster A

Structure-property relationship of Nanocomposites based on Polylactide and Layered Double Hydroxide — •Purv Purohit and Andreas Schönhals — BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany

Nanocomposites based on biopolymer Polylactide (PLA) and organically modified MgAl Layered Double Hydroxide (MgAl-LDH) were prepared and investigated by a combination of differential scanning calorimetry (DSC), Small and Wide angle X-ray scattering (SAXS & WAXS) and Dielectric Relaxation Spectroscopy (DRS). DSC and WAXS show that the degree of crystallinity is influenced by the content of LDH. The dielectric response of the nanocomposites shows several relaxation processes. The intensity of the dynamic glass transition increases with the concentration of LDH. This is attributed to the increasing concentration of the exchanged anion sodium dodecylbenzene sulfonate (SDBS), which are adsorbed at the LDH layers. Two processes are identified at lower and higher temperatures both having a signature of the dynamic glass transition. The process at lower temperature originates from polymer segments close to the LDH whereas the one at higher temperature (bulk like) from the molecules at a farther distance from the LDH. Other than these two processes, β relaxation is identified which is related to localized fluctuations in the polymer chain.

CPP 8.36 Mon 17:30 Poster A

Electrical investigation of gold nanoparticles using heterojunctions based on strained nanomembranes — •Maria Bendova[1], Carlos Cesar Bof Bufon[1], Sandeep Gorantla[2], Mark H. Rümmeli[2], and Oliver G. Schmidt[1] — [1]Institute for Integrative Nanosciences, IFW Dresden, Germany — [2]Institute for Solid State Research, IFW Dresden, Germany

In this work we present the investigation of electrical transport across mono-/bilayers of capped Au nanoparticles (NPs) vertically contacted using strained nanomembranes [1]. The fabrication process consists of a strained Au nanomembrane which rolls up on top of a metal finger structure where the NPs layer was previously deposited. The strained nanomembrane-based electrode provides a soft yet robust contact on top of NPs. The fabrication process is compatible with standard microfabrication techniques and several devices can be created in parallel on a chip. This represents an advantage when compared with other contacting methods (STM, nanogap electrodes).

The transport measurements exhibit Coulomb blockade and Coulomb staircase behavior at 4 K, which is correlated with NPs size and the presence of organic tunneling barriers. The Coulomb peaks in the differential conductance spectra vanish above 50-70 K as the thermal energy exceeds the NPs charging energy. Thus, this method can be directly employed to contact various types of nanoparticulate materials, whereas averaged properties of a macroscopic set of NPs (areas of μm^2) can be obtained.

[1] C. C. B. Bufon et al., *Nano Lett.*, **2011**, 11, 3727.

CPP 8.37 Mon 17:30 Poster A

Förster resonance energy transfer (FRET) experiments on tubular J-aggregates wrapped with dye labeled polyelectrolytes — •Omar Al-Khatib[1], Christoph Böttcher[2], Hans von Berlepsch[2], Jürgen P. Rabe[1], and Stefan Kirstein[1] — [1]HU Berlin, Inst. für Physik Newtonstr. 15, 12489 Berlin — [2]FU Berlin, Forschungszentrum für Elektronenmikroskopie, Fabeckstr. 36a, 14195 Berlin

In this contribution we demonstrate the coating of tubular J-aggregates with dye-labeled polyelectrolytes. The tubular J-aggregates are formed by an amphiphilic cyanine dye in aqueous solutions [1]. These aggregates can be considered as cylindrical objects with 13 nm diameter, length exceeding microns and a negative surface potential. It is shown by cryogenic electron microscopy (cryo-TEM) that polycations can be adsorbed at the aggregate surface forming a homogeneous coating layer. Poly(diallyldimethyl ammonium chloride) (PDAC) and poly(allylamine hydrochloride) (PAH) labelled with different fluorescent dyes are used, acting as donors or acceptors within a Förster energy transfer (FRET) process. The donor and acceptor dyes are distributed homogeneously within the coating. The FRET is investigated by static optical absorption and fluorescence spectroscopy. The experiments demonstrate the possibility for symmetric energy transfer from donors to the aggregate and from the aggregate to acceptors. No indication for enhanced energy transfer due to exciton diffusion was found. [1] D.M. Eisele, et al., Nature Nanotech. 4 (2009) 658;

CPP 8.38 Mon 17:30 Poster A

In-situ sputter deposition: from early stages to final layer growth as seen by in-situ GISAXS — •Stephan V. Roth[1], Ralph Doehrmann[1], Gerd Herzog[1], Gunthard Benecke[1,2], Stephan Botta[1], Adeline Buffet[1], Berit Heidmann[1], Rainer Gehrke[1], Matthias Schwartzkopf[1,3], Ezzeldin Metwalli[4], and Peter Mueller-Buschbaum[4] — [1]DESY, Notkestr. 85, D-22607 Hamburg — [2]MPIKG, Dep. Biomat., Am Mühlenberg 1, D-14424 Potsdam-Golm — [3]Univ. Hamburg, Inst. Techn. Makromol. Chem., Bundesstr. 45 , D- 20146 Hamburg, — [4]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, D-85748 Garching

Understanding the growth kinetics of metal polymer nanocomposites is of utmost importance to tailor the structure-function relationship for materials in modern technologies [1]. The key point during the processing of these nanocomposites is the interaction between the metal atoms and the underlying polymer layer(s) [2,3]. As sputter deposition is one of the most widely used industrial methods for rapid metal coating, we investigate the gold layer growth on top of a thin, spin-coated polystyrene film in-situ using microbeam grazing incidence small-angle x-ray scattering (μGISAXS) with high temporal resolution. We follow the different stages of nanoparticle formation from the initial correlated roughness changes induced by deposition to the fully established layer. We present the full morphological and structural characterization as function of deposition time and gold layer thickness.

[1] Faupel et al., Adv. Eng. Mat. 12, 1177 (2010); [2] Metwalli et al., Langmuir 24, 4265 (2008); [3] Buffet et al., Langmuir 27, 343 (2011)

CPP 8.39 Mon 17:30 Poster A

Density Matrix Description of Molecule Metal Nanoparticle Interactions — •Gerold Kyas, Yaroslav Zelinskyy, Yuan Zhang, and Volkhard May — Institut für Physik, Humboldt-Universität zu Berlin, Germany

Within the emerging field of plasmonics, particular efforts are undertaken to gain a fundamental insight into the interaction between molecules and metal nanoparticles (MNPs). Recent experimental and theoretical studies demonstrated a versatile enhancement effect of the metal supporting various molecular processes, such as light absorption, emission and intermolecular charge and energy transfer. In our approach, we describe these phenomena via a density matrix based microscopic theory, which, in contrast to the proposals made in other works, is fully quantum mechanical and hence free of the need to calculate local electric fields.

As an application, we present a consideration of MNP affected intermolecular excitation energy transfer [1]. Moreover, the emission and absorption spectra of molecular complexes placed in close vicinity to an MNP are discussed [2]. Finally, we briefly comment on plasmon assisted charge transmission through a molecular junction.

[1] G. Kyas and V. May, J. Chem. Phys. 134, 034701 (2011).
[2] Ya. R. Zelinskyy and V. May, Chem. Phys. Lett. 511, 372 (2011).

CPP 8.40 Mon 17:30 Poster A

Modified Guest Chains in Dense Polymer Brushes — •Dirk Romeis[1,2], Holger Merlitz[1,3], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung e.V., 01069 Dresden — [2]TU Dresden, Fachbereich Physik, 01062 Dresden — [3]Department of Physics and ITPA, Xiamen University, Xiamen 361005, P. R. China

Using a quasi off-lattice self-consistent field approach we systematically study the behavior of modified guest chains in densely grafted polymer brushes. The presented approach accounts for finite extensible chains of spherically shaped monomers and the Carnahan-Starling equation of state for hard spheres is applied. Recent MD simulations [1] found significant conformational instabilities for the guest chains, which could be reproduced in quantitative agreement. A simple analytical model is developed, which confirms the encountered scaling laws for the observed conformational transition.
[1] Merlitz H. et. al. [*Macromolecules* **41** 5070, 2008].

CPP 8.41 Mon 17:30 Poster A

Photo-fluorescence spectroscopy of a novel form of ultrastable silicon nanoparticles — Hanieh Yazdanfar, Gediminas Galinis, Gauthier Torricelli, Mark Watkins, Atea Akraiam, and •Klaus von Haeften — Department of Physics and Astronomy, University of Leicester, Leicester, LE1 7RH, United Kingdom

Silicon nanoparticles produced by a novel co-deposition technique [1] show a number of extraordinary properties: clusters smaller than 3 nm in diameter form a stable phase in water, do not agglomerate [2] and emit strong and exceptionally stable fluorescence when excited with UV light [3]. An unequivocal assignment of the fluorescence is challenging because of the breadth of possible geometric structures and cluster sizes. We found the fluorescence wavelength un-shifted irrespective of the excitation energy and concluded that the fluorescent transitions originated from localised defects presumably caused by a chemical reaction of silicon with water. In alcoholic solvents the clusters fluoresce as well but the bands exhibit a blue-shift which we found to correlate with the dipole moment of the solvent molecules and which we interpreted as evidence for a location of the defects at the cluster surface. Size effects were investigated by AFM of clusters placed on HOPG in UHV and by filtering the solutions, which revealed that the fluorescence stemmed only from the smaller clusters in the solution.
[1] K. von Haeften et al. Eur. Phys. J. D 52, 11 (2009).
[2] A. Brewer, K. von Haeften, Appl. Phys. Lett. 94, 261102 (2009).
[3] G. Torricelli, A. Akraiam, K. von Haeften, Nanotechnology 22, 315711 (2011).

CPP 8.42 Mon 17:30 Poster A

Tailoring the blinking behaviour of single CdSe/ZnS nanoparticles — •Daniel Braam, Andreas Mölleken, Günther M. Prinz, Martin Geller, and Axel Lorke — Fakultät für Physik and CeNIDE, University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany

Though CdSe/ZnS nanoparticles have been investigated over the last decades, their emissive behaviour still lacks a complete understanding. Single particle photoluminescence (PL) measurements have the ability to give insight into the underlying recombination processes. With a custom-built μ-PL setup, using a LN$_2$ cooled CCD-camera attached to an imaging spectrometer, we can aquire time-resolved 2D-images of several nanoparticles to investigate them and their blinking statistics simultaneously. Specific particles can be selected for further spectral characterisation. Here, we focus on the influence of different rough metal layers on the brightness and stability of the luminescence. We observe intensity enhancement, which we attribute to plasmonic effects, and continuous blue shifts of several tens of nanometers during illumination, which is accompanied by randomly varying stark shifts. At low temperatures ($\leq$10 K) some particles show spectral jumps of 25 meV instead of blinking, which indicate altered radiative and nonradiative recombination rates induced by the aluminium layer.

CPP 8.43 Mon 17:30 Poster A

Functionalized Luminescent Silicon Quantum Dots — •Marc Wegmann, Georg Brehm, and Carola Kryschi — Friedrich-Alexander University of Erlangen, Egerlandstr. 3, 91058 Erlangen, Germany

One of the central challenges in fabrication of luminescent Si quantum dots (SiQDs) tailored for nano-optolelectronics is to functionalize their surfaces with electronically efficiently coupled molecules that mediate carrier injection into the bulk and allow to optically control charge separation as well as luminescence properties of the bulk. In this contribution we will present a detailed spectroscopy study of bright green-luminescent alkenyl-passivated SiQDs with were prepared via a four-step wet-chemistry synthesis route. The sizes, cristallinity and shapes as well as the surface structures of differently functionalized SiQDs were examined employing high-resolution transmission electron microscopy (HRTEM) and FTIR spectroscopy, respectively. Stationary and time-resolved photoluminescence spectroscopy experiments provided essential information of luminescent surface and bulk states. The interplay between electronically excited molecular states and conduction band states was examined upon directly monitoring photo-excited carrier dynamics with femtosecond transient absorption and luminescence up conversion spectroscopy.

CPP 8.44 Mon 17:30 Poster A

Concave Micro/Nanoparticles as Powerful Facilitators for Bonding of Non-Adhesive Polymers — •Xin Jin[1], Sebastian Wille[1], Dawit Gedamu[1], Rainer Adelung[1], Jan Strüben[2], Anne Staubitz[2], Lars Heepe[3], Alexander Kovalev[3], and Stanislav Gorb[3] — [1]Functional Nanomaterials, Institute for Materials Science, University of Kiel — [2]Otto-Diels Institute of Organic Chemistry, University of Kiel — [3]Functional Morphology and Biomechanics, Institute of Zoology, University of Kiel

Modern engineering often requires that two polymer objects are firmly joined together, while at the same time demanding that specific properties and functions of each individual polymer are preserved. In many cases, chemical and mechanical properties of polymers to be joined are so different that strong adhesive bond between them by using conventional methods is hardly possible. In this work, we present a new approach to facilitate strong adhesion between non-adhesive polymers, such as PTFE and crosslinked PDMS, by employing tetrapod ZnO micro/nanoparticles with concave cross-section. We show that the adhesion force attained by this approach is of the same order of magnitude as obtained by plasma etching method and can be seen as a viable, simple alternative to this method. The tetrapod micro/nanoparticles were produced in high quantities at low cost with Flame Transport Synthesis(FTS). Results from peeling tests, SEM observations, and video recordings of peeling process are presented. The mechanisms of adhesion enhancement are discussed in detail. Acknowledgement: We thank DFG SFB677-C10 for the financial support.

CPP 8.45 Mon 17:30 Poster A

Transmission electron microscopy investigation of a gold / TiO$_2$ catalyst — •Kristian Frank, Andre Wichmann, Arne Wittstock, Lutz Mädler, Marcus Bäumer, and Andreas Rosenauer — Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

Nanoporous gold is a material for many applications e.g. in catalysts, sensors and electrode materials. It is created by chemical etching of a gold - silver alloy. Important structural properties are the pore size and the size of the gold ligaments. For the application in catalysis of CO-oxidation, the gold can be coated with TiO$_2$ in order to enhance catalytic activity. In the temperature range above 60 °C the CO conversion of the TiO$_2$ coated sample is increased by more than one order of magnitude compared with the pure nanoporous gold. The structure and distribution of the TiO$_2$ on the gold surface is an important property, which was investigated by TEM. It was shown, that the gold ligaments are abundantly covered by approximately 5 nm TiO$_2$ particles. The determination of the largest lattice fringe distance with HR-TEM revealed that the crystalline nanoparticles consist of the anatase phase. The spatial Ti distribution was measured with EFTEM (energy filtered TEM).

CPP 8.46 Mon 17:30 Poster A

The ordering of dodecyl chains and their influence on the agglomeration of zirconia nanoparticles — •Silvia Pabisch[1], Bernhard Feichtenschlager[2], Guido Kickelbick[3], and Herwig Peterlik[1] — [1]University of Vienna, Faculty of Physics, Vienna, Austria — [2]Vienna University of Technology, Institute for Materials Chemistry, Vienna, Austria — [3]Saarland University, Inorganic Solid State Chemistry, Saarbrücken, Germany

The ordering of dodecyl chains has been investigated in mixed monolayers of phosphonic acid capping agents on the surface of hydrothermal prepared zirconia nanocrystals. As co-capping agent for the mixed monolayer formation, methyl-, phenyl-, pyryl- and tert-butyl phosphonic acid have been used to investigate series with different mixing ratios with dodecyl phosphonic acid. In this study, the influence of the various molecules on the alkyl chain disordering is discussed. Small angle X-ray scattering (SAXS) studies show that with increasing amount of co-capping agent the agglomeration of the particles decreases. This behavior correlates with the ordering of the surface bond alkyl chains investigated by Fourier transform infrared spectroscopy (FTIR). It can be concluded that interparticle bilayers, formed via long alkyl chain packing, are responsible for the formation of dense particle agglomerates and can be controlled on a molecular level by co-adsorbing various molecules. Based on this correlation nanoparticles can be used as probes for self-assembled monolayer investigation by an indirect method (SAXS) and correlated with the routine method for the chemical analysis of surface groups (FTIR).

CPP 8.47 Mon 17:30 Poster A

AFM investigations of surface properties of 2, 4, 6 trinitrophenol (TNP) crystal at the nanoscale — •Alexander Kovalev[1] and Heinz Sturm[1,2] — [1]BAM - Fed. Inst. Materials Res. - Div. Nanotribology and Nanostructuring, 12205 Berlin — [2]TU Berlin, IWF, 10587 Berlin

Knowledge of the behaviour of energetic materials (EM) subjected to phenomena at the nanometre scale is a main key to better understanding the nature of initiation processes of an explosion. The chemical-mechanical decomposition of EM is not fully understood, and the initial decomposition steps are not firmly established, but the model of hotspot formation is generally accepted. The initial size of a hotspot is comparable with molecular dimensions of EM. It is evident that the real origin of ignition should be explored at the nanometre scale, and such possibility are provided by atomic-force microscopy (AFM) techniques. Here, we report on the direct initiation of the hotspot formation on surfaces of 2, 4, 6-trinitrophenol (TNP) single crystals by the AFM tip. The immediate AFM imaging of the selected region revealed the destructive changes of TNP crystals, and allows a first estimate of the evolution of hotspot phenomenon at the initial stage. The direct observation of the nanoscale surface restructuring of TNP crystal during the AFM scanning has been explored. Our results reveal the instability of TNP molecules at the border of molecular layers at normal ambient condition. Based on the explored properties of TNP crystal a mechanism of hotspot formation at the nanoscale is proposed.

CPP 8.48 Mon 17:30 Poster A

Probing nanomechanical structure-property relationships of micro- and nanofibers by AFM bending experiments — Daniel Kluge and •Andreas Fery — Physikalische Chemie II, Universität Bayreuth, Universitätsstraße 30, 95440 Bayreuth, Germany

Micro- and nanofibers are important structural elements in biomaterials and tissues, where one of their main functions is providing mechanical stability. Characterizing these small-scale fibers requires highly specialized techniques beyond standard methods for macroscopic materials. Nanoscale bending of the fibers is a common approach and applicable for a wide variety of fiber systems.

In our contribution, we focus on bending experiments of fibers suspended over channels: We show results on bending perpendicular and parallel to the substrate plane. We will discuss major advantages of these two bending modes, for example validation of boundary conditions, direct integration of optical methods and detailed investigation of the mechanical properties beyond linear elastic deformations.

Our experiments allow us to investigate the properties of numerous novel materials and we will present in detail our studies on supramolecular benzenetrisamide aggregates. Small changes in their molecular structure can significantly influence their morphology, which makes them suitable for "bottom-up" tailored materials. We look into the effect of the molecular structure on their mechanical behavior and compare benzenetrisamide whiskers and fibers obtained by different preparation methods.

CPP 8.49 Mon 17:30 Poster A

Nuclear Quantum Effects of Liquid Water from First Principles by Force Matching — Christopher John[1], Thomas Spura[1], Scott Habershon[2], •David E. Manolopoulos[2], and Thomas D. Kühne[3] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Staudinger Weg 9, D-55128 Mainz, Germany — [2]Physical and Theoretical Chemistry Laboratory, Oxford University, South Parks Road, Oxford OX1 3QZ, United Kingdom — [3]Institute of Physical Chemistry and Center for Computational Sciences, Johannes Gutenberg University Mainz, Staudinger Weg 9, D-55128 Mainz, Germany

We have applied the ring polymer molecular dynamics (RPMD) method [1,2] to investigate the effects of nuclear quantum effects of liquid water from first principles. Due to the fact that direct ab-initio RPMD simulations would be computational far too expensive, a flexible water potential is parameterized on forces from DFT-based Car-Parrinello-like MD simulations [3]. Initial results of RPMD simulations to determine static as well as dynamic properties of liquid water at ambient conditions using the so derived effective potential are presented and the importance of nuclear quantum effects are discussed.

[1] I. R. Craig and D. E. Manolopoulos, J. Chem. Phys. 121, 3368 (2004).

[2] B. J. Braams and D. E. Manolopoulos, J. Chem. Phys. 125, 124105 (2006).

[3] T. D. Kühne, M. Krack, F. R. Mohamed and M. Parrinello, Phys. Rev. Lett. 98, 066401 (2007).

CPP 8.50 Mon 17:30 Poster A

Nuclear Quantum Effects of Liquid Water from First Principles by Force Matching — Christopher John[1], Thomas Spura[1], Scott Habershon[2], •David E. Manolopoulos[2], and Thomas D. Kühne[3] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Staudinger Weg 9, D-55128 Mainz, Germany — [2]Physical and Theoretical Chemistry Laboratory, Oxford University, South Parks Road, Oxford OX1 3QZ, United Kingdom — [3]Institute of Physical Chemistry and Center for Computational Sciences, Johannes Gutenberg University Mainz, Staudinger Weg 9, D-55128 Mainz, Germany

We have applied the ring polymer molecular dynamics (RPMD) method [1,2] to investigate the effects of nuclear quantum effects of liquid water from first principles. Due to the fact that direct ab-initio RPMD simulations would be computational far too expensive, a flexible water potential is parameterized on forces from DFT-based Car-Parrinello-like MD simulations [3]. Initial results of RPMD simulations to determine static as well as dynamic properties of liquid water at ambient conditions using the so derived effective potential are presented and the importance of nuclear quantum effects are discussed.

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[2] B. J. Braams and D. E. Manolopoulos, J. Chem. Phys. 125, 124105 (2006).

[3] T. D. Kühne, M. Krack, F. R. Mohamed and M. Parrinello, Phys. Rev. Lett. 98, 066401 (2007).

CPP 9: Biopolymers and Biomaterials (joint session with BP)

Time: Tuesday 9:30–13:00 Location: H 1058

Invited Talk CPP 9.1 Tue 9:30 H 1058

Surface topology effect on cell interaction at the nanoscale — •Giuseppe Battaglia — Department of Biomedical Science, The University of Sheffield, Sheffield, UK

One of the most important classes of synthetic systems for creating self-assembled nanostructures is amphiphilic block copolymers. By controlling the architecture of individual molecules, it is possible to generate nanostructures either in an undiluted melt or in solution. These ordered nanostructures are tunable over a broad variety of morphologies, ranging from discrete micelles and vesicles to continuous network structures. Their synthetic nature allows the design of interfaces with different chemical functional groups and geometrical properties. This, in combination with molecular architecture, determines the levels of ordering in self-organizing polymeric materials. Such an effective control is extremely beneficial when it comes to design materials that have to interact with biological systems. I will be discussing how block copolymers can be used for the design of nanoscopic vectors that go across different biological barriers from the thick tissues to the very cell interior to deliver therapeutic agents and/or diagnostic probes. Similarly exploiting the facile interface engineering of block copolymers I will show how these can be used to design functional interfaces for polymeric scaffolds for cell and tissue engineering.

CPP 9.2 Tue 10:00 H 1058

Molecularly imprinted conductive polymers for controlled trafficking of neurotransmitter at solid-liquid interfaces — •Neelima Paul[1,2], Markus Mueller[1], Amitesh Paul[3], Elke Guenther[4], Iver Lauermann[1], Peter Müller-Buschbaum[2], and Martha Ch. Lux-Steiner[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85747 Garching, Germany — [3]TU München, Physik-Department, LS Neutronenstreuung, James-Franck-Str. 1, 85748 Garching, Germany — [4]Natural and Medical Sciences Institute at the University of Tübingen, Markwiesenstr. 55, 72770 Reutlingen, Germany

The state of the art approach to restore sight in certain cases of blindness is the replacement of the damaged photoreceptors by a subretinal implant consisting of light-sensitive photodiodes . We suggest to chemically stimulate the neurons by replacing the photodiodes in the subretinal implant by a molecularly imprinted polymer (MIP), imprinted with a neurotransmitter, such as glutamate. By controlling the neurotransmitter trafficking across a solid-liquid interface with voltage, we show the possibility of using this MIP for chemical stimulation of retinal neurons. ATR-FTIR spectroscopy and XPS has been used to chemically confirm the imprint of neurotransmitter in the MIP at the solid-liquid and the solid-air interface respectively. Fluorescence spectroscopy using the dye, fluorescamine, has been used to monitor the changes in neurotransmitter concentration in various solvents.

CPP 9.3 Tue 10:15 H 1058

Excitation energy transfer processes in coupled phycobiliprotein complexes of A. marina and semiconductor nanocrystals forming hybrid structures — •Franz-Josef Schmitt[1], Evgeny Maximov[3], Patrick Hätti[2], Vithiya Jeyasangar[2], Jörn Weissenborn[2], Vladimir Paschenko[3], Hans Joachim Eichler[2], Thomas Friedrich[1], and Gernot Renger[1] — [1]Max Volmer Laboratory for Biophysical Chemistry — [2]Institute of Optics and Atomic Physics, Berlin Institute of Technology, Germany — [3]Department of Biophysics, M.V. Lomonosow Moscow State University, Russia

Pigment-protein complexes isolated from the photosynthetic apparatus provide functionally optimized nanoscaled devices for the construction of light driven operational units. The present work describes results obtained on hybrid systems consisting of CdSe quantum dots (QDs) with ZnS shell and different phycobiliproteins (PBPs) like hexameric phycoerythrin (PE), phycocyanin (PC), allophycocyanin (APC) and rod shaped PBP antenna complexes from the cyanobacterium Acaryochloris marina. The surface of the QDs is functionalised by covering with anionic and cationic groups leading to electrostatic contact with PBP. Excitation energy transfer (EET) from QDs to PBPs occurs with varying efficiency of up to 90 % for coupled QD/PBP hybrid complexes and is highly dependent on the temperature. The study with different QDs shows that the Förster Integral crucially determines the efficiency of EET while the electrostatic surface charge is of secondary relevance. Highly efficient EET and fluorescence enhancement of the acceptor was observed for particular stoichiometric ratios between QDs and PBPs.

CPP 9.4 Tue 10:30 H 1058

Neutron radiography study of water migration into casein micellar films — •Ezzeldin Metwalli[1], Helen E. Hermes[2], Elbio Calzada[3], Stefan U. Egelhaaf[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany — [2]Physik der weichen Materie, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany — [3]Forschungsneutronenquelle Heinz Maier-Leibnitz, TU München, 85747 Garching, Germany

Casein, a milk protein, forms micelles with a radius of about 100-300 nm. Casein-protein based films are widely used as an adhesive for labeling glass bottles and other containers because of their superior mechanical stabilities in different humidities at temperatures between 2 and 40 C. This study demonstrates the use of neutron radiography as a viable method for the determination of the diffusion profile of water in casein films. The dry casein film is contacted with water and neutron radiographs are collected as function of elapsed time. Profiles of the water concentration are successfully measured by imaging. Two diffusion processes are observed: (a) fast diffusion with a decaying diffusion constant, resulting from water exchange with the hydration water bound to the casein proteins, and (b) slow and constant diffusion due to Fickian water transport into the voids and holes between the casein micelles and their aggregates in the porous film. Time evolution of the later diffusion process is compared with our recent GISANS investigation [1] of hydration behavior of casein thin films in water vapor. [1] Metwalli et al., Langmuir 25, 4124 (2009)

CPP 9.5 Tue 10:45 H 1058

Study of lipid and protein coatings on titanium surfaces by neutron scattering — •Maksym Golub[1], Regine Willumeit[1], Berengere Luthringer[1], Frank Feyerabend[1], Eric Watkins[2], Dieter Lott[1], Vasyl Haramus[1], Boris Toperveg[3], and Andreas Schreyer[1] — [1]Helmholtz Zentrum Geesthacht, Geesthacht, Germany — [2]ILL, Grenoble, France — [3]Ruhr-University Bochum, Germany

Permanent implants, e.g. using titanium and its alloy, are widely used and successfully implemented in medicine. To improve their performance lipid*s covering is applied. The study of the structure of the phospholipid (palmitoyl-oleoyl-sn-glycero-3-phosphoethanolamine - POPE) layering under liquid conditions in presence of growth medium and Human Serum Albumin (HSA), which is the favourable condition for cell adhesion, would provide key parameters to understand the interaction between cells and lipid coated implants. Such a system was measured by neutron reflectivity. Silicon crystals with a Ti layer (36 nm) on the top were covered by POPE lipids and measured at different conditions: D2O, D2O based growth medium and growth medium with protein i.e., HSA. A 2D detector was used for the data collection which allowed us to detect also the diffuse scattering which provides information about the lateral correlations in these films. The neutron reflectivity experiments enabled us to see the changes of layer structure due to adhesion of the protein and will be discussed here in detail.

CPP 9.6 Tue 11:00 H 1058

Adhesion of gecko setae reflects nanoscale differences in subsurface energy — •Peter Loskill[1], Jonathan Puthoff[2], Matt Wilkinson[2], Kellar Autumn[2], and Karin Jacobs[1] — [1]Saarland University, Experimental Physics, D-66041 Saarbrücken, Germany — [2]Department of Biology, Lewis & Clark College, Portland, OR 97219, USA

Surface energies are commonly employed to determine the adhesive forces between materials. However, the component of surface energy derived from long-range forces, such as van der Waals forces, depends on the material's structure below the outermost atomic layers. Prior theoretical results and indirect experimental evidence suggest that the van der Waals energies of subsurface layers will influence interfacial adhesion forces. We discovered that nanometerscale differences in the oxide layer thickness of silicon wafers result in significant macroscale differences in the adhesion of isolated gecko setal arrays. Si/SiO_2 bilayer materials exhibited stronger adhesion when the SiO_2 layer is thin (approx. 2 nm). To further explore how layered materials influence adhesion, we functionalized similar substrates with an OTS monolayer and again identified a significant influence of the oxide layer thickness on adhesion. Our theoretical calculations describe how variation in the silicon dioxide layer thickness produces differences in the van der Waals interaction potential, and these differences are reflected in the adhesion mechanics. Setal arrays employed as tribological probes provide the first empirical evidence that the 'subsurface energy' of inhomogeneous materials influences the macroscopic surface forces.

15 min break

CPP 9.7 Tue 11:30 H 1058

Biocompatibility of $Fe_{70}Pd_{30}$ ferromagnetic shape memory films for cell actuation — •Uta Allenstein[1], Yanhong Ma[2], Ariyan Arabi-Hashemi[2], Stefan G. Mayr[2], and Mareike Zink[1] — [1]Division of Soft Matter Physics, Institute for Experimental Physics I, University of Leipzig, Germany — [2]Leibniz-Institut für Oberflächenmodifizierung e.V., Translationszentrum für Regenerative Medizin and Fakultät für Physik und Geowissenschaften, Universität Leipzig, Germany

Ferromagnetic shape memory alloys (FSMAs) are a very promising and highly applicable class of smart functional materials which show various interesting features, such as the induction of large reversible strains of several percent due to an external magnetic field at a moderate stress. These properties support the application as actuators or valves in biomedical devices, as well as bone prostheses. Of course in vivo implantation demands good biocompatibility and adhesion of different tissues to the material. Thus, our study investigated the cellular response in contact with single crystalline $Fe_{70}Pd_{30}$ FSMA films on MgO substrates. The adhesive properties as well as the viability and proliferation of different cell types where tested on the substrates and tuned by coating the substrates with different adhesive materials, such as Fibronectin, Laminin and Poly-L-Lysin. Tests were carried out with NIH 3T3 mouse fibroblasts, MCF 10A human epithelial cells and primary HOB human osteoblasts. We show that these three cell types obtain the ability to adhere and proliferate well on $Fe_{70}Pd_{30}$ FSMA substrates, demonstrating good biocompatibility of the films.

CPP 9.8 Tue 11:45 H 1058

Direct Laser Writing for Three-dimensional Biological Application — •Benjamin Richter[1,2], Alexandra Greiner[1], Clemens Franz[1,2], Martin Wegener[2,3,4], and Martin Bastmeyer[1,2] — [1]Zoologisches Institut, Karlsruher Institut für Technologie, 76131 Karlsruhe — [2]DFG-Center for Functional Nanostructures (CFN), Karlsruher Institut für Technologie, 76131 Karlsruhe — [3]Angewandte Physik, Karlsruher Institut für Technologie, 76131 Karlsruhe — [4]Institut für Nanotechnologie, Karlsruher Institut für Technologie, 76021 Karlsruhe

Direct laser writing (DLW) is a versatile technique to fabricate tailored three-dimensional (3D) cell-culture scaffolds in the micrometer to nanometer range. By sequential DLW of two different photoresists, composite-polymer scaffolds with distinct protein-binding properties are fabricated and selectively bio-functionalized thereafter. Cells cultured in these scaffolds selectively form cell-adhesion sites with the functionalized parts, allowing for controlling cell adhesion and cell shape in 3D * forming the basis for future designer tissue-culture scaffolds. To go one step further photoactivation of 3D scaffolds might play an important role in the future. One application realized by using these two-component polymer scaffolds is measuring forces of cells in a three-dimensional environment. With our technique we can control the number, size, and geometry of adhesive cubes. The forces induced by a single cell onto the scaffolds are proportional to the bending of the beams.

CPP 9.9 Tue 12:00 H 1058

Superparamagnetic Iron Oxide Nanoparticles as Radiosensitizer for Radiation Therapy — •Anja Sommer[1], Stefanie Klein[1], Luitpold Distel[2], and Carola Kryschi[1] — [1]Department of Chemistry and Pharmacy, Institute of Physical Chemistry I, University of Erlangen, Egerlandstr. 3, 91058 Erlangen, Germany — [2]Department of Radiation Oncology, University of Erlangen, Universitaetsstr. 27, 91058 Erlangen, Germany

Superparamagnetic iron oxide nanoparticles (SPION) have been widely used experimentally for numerous in vivo applications such as magnetic resonance imaging (MRI) contrast enhancement, hyperthermia and targeted drug delivery. we present the synthesis of surface-stabilized ultrasmall superparamagnetic iron oxide nanoparticles. In this contribution, we will report on functionalized SPION with sizes between 4 and 15 nm which were synthesized by alkine coprecipitation or thermal decomposition and subsequently coated with biocompatible acids. The differently stabilized SPION were fully characterized using HRTEM, XRD, SQUID, FTIR and Raman spectroscopy, XPS, TGA-MS and TGA-IR coupling and zeta potential measurements. Furthermore we present studies about their biocompatibility for cancer cell lines and their potential as radiosensitizer in radiation therapy.

CPP 9.10 Tue 12:15 H 1058

X-ray diffraction on biocomposite materials at high hydrostatic pressure — •Christina Krywka[1], Roxana Ene[2], Shin-Gyu Kang[3], and Martin Müller[3] — [1]Christian-Albrechts-Universität zu Kiel, Institut für Experimentelle und Angewandte Physik, Leibnizstr. 19, D-24098 Kiel — [2]Universität Leipzig, Fakultät für Physik und Geowissenschaften, Linnéstr. 5, 04103 Leipzig — [3]Helmholtz Zentrum Geesthacht, Max-Planck-Str. 1, D-21502 Geesthacht

The anisotropic compressibilites of the crystalline fractions of biocomposite materials (spider silk, silkworm silk, cellulose etc.) were analysed using wide angle X-ray scattering (WAXS) at moderate high pressure (0.01 to 0.5 GPa) using a hydrostatic high pressure cell. With this method, the compression moduli of the biocomposite materials were determined for the first time with high pressure resolution in a pressure range that corresponds to loads as they occur under natural conditions. Exemplarily, for spider silk the compression modulus of the nanocrystals is proven to be highest in the direction of intra-sheet hydrogen bonds. In addition, it is found that the applied pressure may increase the organization of the amorphous phase, indicated by a pressure enhanced diffraction ring.

CPP 9.11 Tue 12:30 H 1058

Subspecies of nacre protein "perlucin" favors binding to aragonite over binding to calcite microcrystals — •Hanna Rademaker, Malte Launspach, and Monika Fritz — Institute for Biophysics, University of Bremen, Germany

Nacre is a compound material of calcium carbonate platelets and organic layers of chitin and proteins. The outstanding mechanical properties of nacre make it desirable to understand the details of the biomineralizing process. The calcium carbonate platelets in nacre show the crystal structure of aragonite and not of calcite. Therefore we are especially interested in proteins which favor binding to aragonite over binding to calcite. We adapted a simple detection method from Suzuki et al. [1] for this purpose.

In this work [2] biomineralizing proteins were chemically removed from the acid-insoluble matrix of nacre from *Haliotis laevigata* and incubated with aragonite and calcite microcrystals, respectively. The crystals were washed and then dissolved. SDS-PAGE of these solutions showed that one protein, a subspecies of perlucin, favors binding to aragonite crystals. This might be a hint that perlucin plays a key role in the biomineralization process.

[1] M. Suzuki et al., Science, **325** (5946), 1388-1390, 2009

[2] H. Rademaker and M. Launspach, Beilstein J. Nanotechnol., **2**, 222-227, 2011

CPP 9.12 Tue 12:45 H 1058

Assessment of swelling driven actuation in a two-phase cellular material — •Lorenzo Guiducci[1], Yves J. M. Brechet[2], Peter Fratzl[1], and John W. C. Dunlop[1] — [1]Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, Am Mühlenberg 1, Science Park Golm, Potsdam, Germany — [2]SIMaP-Grenoble Institute of Technology, Saint Martin d'Hères, France

Natural systems that are able to actuate -that is, generate stress/strain- have recently drawn the attention of scientific community. Examples include the seed dispersal unit of the wild wheat and stork's bill awn, which are able to crawl on the ground following the daily humidity cycle and the hydro-actuated unfolding of the ice-plant seed capsule.

In natural actuators, the extent of max elongation/forces depends on underlying microstructure, and swelling properties of the constituents: here we present a finite element (FE) simulation study that aims to assess the actuation performance -eigenstrains and effective stiffness at a certain swelling level- of an ideal two-phase cellular material. The eigenstrains assessment is rigorously performed simulating a tessellation of the bidimensional space with given unit cell. As observed in preliminary simulations of a finite patch of material with free boundaries, the resulting two-phase material deforms in a highly anisotropic way. For each value of swelling pressure, we get an equilibrated configuration of the unit cell that becomes the starting point for the calculation of the effective mechanical properties. Finally, we show that the FE results can be understood in terms of a simpler lattice spring model.

CPP 10: Interfaces and Thin Films II

Time: Tuesday 9:30–13:00 Location: C 130

Topical Talk CPP 10.1 Tue 9:30 C 130

PEG Functionalized Lipid Bilayers at the Solid / Liquid Interface: Protrusions versus Blisters — •Beate Klösgen[1], Giovanna Fragneto[2], Avi Halperin[3], Ole G. Mouritsen[1], Patricia Hardas[4], and Michele Sferrazza[4] — [1]University of Southern Denmark, Odense, Denmark — [2]Institute Laue-Langevin, Grenoble, France — [3]Université Joseph Fourier, Grenoble, France — [4]Université Libre de Bruxelles, Bruxelles, Belgique

PEGylated lipids inoculated into fluid membranes constitute a membrane disturbance due to conformational restrictions of the polymer when grafted to the membrane interface. Blisters and protrusions were both discussed as possible responses to the hydrophilic pull. Neutron reflectivity of adsorbed lipid membranes at the solid/water interface supports the protrusion model. Results are shown from an asymmetric system with an inner leaflet consisting of 1,2-distearoyl-sn-glycero-3-phosphorylcholine (DSPC) and an outer leaflet composed of DSPC and Polyethylene glycol (PEG) functionalized 1,2-distearoyl-sn-glycero-3-phosphoethanolamine (DSPE-PEG). DSPC headgroups were deuterated to enhance sensitivity and mark the lipid headgroup/water interface. A narrow water layer at the inner interface allows for some membrane deformation, equally found for the outer headgroup layer in the absence of polymer. This roughness is enhanced when PEG chains are present; the roughness of the inner headgroup layer is about constant. The outer headgroup layer roughness increases with PEG-lipid mole fraction and temperature. The findings suggest that PEG chains favour headgroup protrusions rather than blister like deformations.

CPP 10.2 Tue 10:00 C 130

Interactions and stability of foam films from oppositely charged polyelectrolyte/surfactant mixtures — •Nora Kristen-Hochrein, Heiko Fauser, Martin Uhlig, and Regine von Klitzing — Stranski-Laboratorium, Institut für Chemie, TU Berlin, Germany

Polyelectrolyte/surfactant mixtures in foams play an important role in many technical applications. To control the properties of the foam it is important to investigate single foam films. A measure of the interactions between the two film interfaces is the disjoining pressure, which is the sum of electrostatic, van der Waals and steric forces. The disjoining pressure as a function of film thickness is measured with a Thin Film Pressure Balance (TFPB). In this study we focus on the influence of negatively charged polyelectrolytes on foam films stabilized with cationic surfactant. At low polyelectrolyte concentrations the charge at the surface is positive. With increasing amount of polyelectrolyte the charge of the complexes is reduced and then reversed. However, surface characterization indicates that no charge reversal occurs at the film interfaces. To test the influence of the polyelectrolyte and surfactant hydrophobicity[1,2], results on the stability of films with different polyelectrolytes and surfactants are shown and compared with surface tension and elasticity and neutron reflectometry measurements.

[1] N. Kristen, V. Simulescu, A. Vüllings, A. Laschewsky, R. Miller and R. v. Klitzing, J. Phys. Chem B (2009) 113 7985.

[2] N. Kristen-Hochrein, A. Laschewsky, R. Miller, R. v. Klitzing, J. Phys. Chem B, (2011) DOI: 10.1021/jp206964k

CPP 10.3 Tue 10:15 C 130

Hydration Interactions between Biological Membranes: Molecular Dynamics Analysis — •Matej Kanduc[1], Emanuel Schneck[2], and Roland Netz[1] — [1]Freie Universität Berlin — [2]Technische Universität München

Interactions between biological surfaces result from the interplay of various physical contributions. Dispersion interactions and screened electrostatics have been successfully treated in a continuum approximation, whereas the so-called hydration interaction caused by water structuring at interfaces, still elude a quantitative description. In fact, the interaction between charge-neutral phospholipid membranes is dominated by this contribution in a wide range of separations. Despite the qualitative agreements of various theories, it has become a consensus view during the last decades that in order to explain the hydration interaction on a quantitative level, the structure of the solvent has to be taken into account explicitly. This insight has drawn the attention towards the application of atomistic simulations, where water molecules are treated explicitly including all relevant degrees of freedom. We introduce a novel thermodynamic extrapolation method that provides greatly improved interaction measurements in Molecular Dynamics simulations. The results are quantitatively compared with classical membrane swelling experiments.

CPP 10.4 Tue 10:30 C 130

Temperature-induced transition from odd-even to even-odd effect in polyelectrolyte multilayers due to interpolyelectrolyte interactions — •Peter Nestler[1], Stephan Block[2], and Christiane A. Helm[1] — [1]Institut für Physik, Uni Greifswald, Felix-Hausdorff-Str. 6, 17487 Greifswald, Germany — [2]ZIK HIKE, Uni Greifswald, Fleischmannstr. 42 - 44, D-17487 Greifswald, Germany

Within a liquid cell the linear growth of polyelectrolyte multilayers by LbL technique is observed using multiple angle null-ellipsometry. Poly(styrenesulfonate) (PSS) and poly(allylamine hydrochloride) (PAH) are used. The salt content is varied between 1 and 4 mol/L NaCl, the temperature between 20 and 55°C. The outermost layer is investigated. At low temperature a top PSS layer is twice as thick as a top PAH layer (odd-even effect), consistent with the respective monomer volume and the same water content for both polyelectrolytes. On heating, the thickness of a polycation/polyanion bilayer increases. For temperatures exceeding T_{x-over} a top PAH layer is thicker than a top PSS layer (even-odd effect). In this case, the index of refraction of the respective top layers indicates a compact PSS and a swollen PAH layer. At temperatures above T_{x-over} the dried films destabilize, an increased roughness and a random pattern of holes is observed. It is suggested that at elevated temperature and high salt-conditions, secondary forces gain importance in comparison to electrostatic forces: therefore a transition from an odd-even to an even-odd effect occurs, as well as the decreased film stability on drying.

CPP 10.5 Tue 10:45 C 130

Diffusion study in thin free-standing liquid crystal films — •Benjamin Schulz and Christian Bahr — MPI für Dynamik und Selbstorganisation, 37077 Göttingen

Free-standing liquid crystal films are liquid films that are spanned over a supporting frame and stable without an underlying substrate. Hence it becomes possible to study the pure material properties in thin films as no surface interaction comes into play. However, not much is known about the changes in diffusion in such films as compared to bulk properties.

We study the translational molecular dynamics in free-standing films using single molecule tracking. For this we dissolve a small amount of dye molecules to then image their diffusive behaviour. This allows us to directly study the dynamics in the film on molecular level. We focus on the diffusion in films at the transition to complete 2-dimensional systems with a thickness of only a few layers, which leads to a strong increase in diffusion for some materials. Also we look into the diffusion properties in proximity to phase transitions as for some materials it is known that they show layer-by-layer phase transitions in the layers directly at the free surface [1].

[1] Jin et. al., Phys. Rev. E. 49 (1994), R4791-R4794

CPP 10.6 Tue 11:00 C 130

Interfacial effects on single dye dynamics in ultrathin liquid and thin liquid crystal films — •Daniela Täuber and Christian von Borczyskowski — nanoMA, TU-Chemnitz, Institut für Physik

Silica surfaces are widely used e.q. in the fabrication of organic electronic devices. Minimization of devices thereby induces strong confinement on the organic compound and thus enhances interfacial effects. Yet many details of the interactions between silica surfaces and organic molecules which are crucial for their electrical properties and thus for device performance are not fully understood. Here we use single molecule methods to explore the dynamics of dye molecules within ultrathin liquid films [1,2] and thin liquid crystal films [3] on differently treated silica surfaces. This allows us to draw conclusions on diffusion coefficients and physio-chemical binding affinities depending on the chemical structure of participating molecules and silica surfaces.

[1] D. Täuber, C. von Borczyskowski et al: Diff. Fund. J. 11 (2009) 76.

[2] D. Täuber, Dissertation, TU Chemnitz, 2011.

[3] B. Schulz, D. Täuber, J. Schuster, T. Baumgärtel, and C. von Bor-

czyskowski, Soft Matter 7 (2011) 7431.

15 min break

CPP 10.7 Tue 11:30 C 130

Coherent acoustic phonon propagation through organic interface layers — •Mike Hettich, Karl Jacob, Martin Schubert, Oliver Ristow, Axel Bruchhausen, and Thomas Dekorsy — Department of Physics and Center of Applied Photonics, Universität Konstanz, D-78457 Konstanz, Germany

The damping of coherent acoustic phonons in thin gold films was investigated by asynchronous optical sampling (ASOPS) [1]. A distinct change of the damping time of the gold film's breathing mode is observed depending on the acoustic phonon frequency, when self assembled molecular layers (SAMs) are introduced at the interface between the film and a substrate [2]. We thoroughly characterized this system by varying the thickness of the organic interface layer from a single monolayer ($\approx$ 0.7nm) up to 12 nm. This allowed the investigation of the elastic properties of the SAMs in a transition regime that highlights the limitations of the elastic-continuum description when reducing the size of the organic interlayer to the nanometer scale.

References
[1] A. Bartels et al., Rev. Sci. Instr. **78**, 035107 (2007)
[2] M. Hettich et al., Appl. Phys. Lett. **98**, 261908 (2011)

CPP 10.8 Tue 11:45 C 130

Phase separation dynamics in a two-dimensional magnetic mixture — •Ken Lichtner[1], Andrew J. Archer[2], and Sabine H. L. Klapp[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Department of Mathematical Sciences, Loughborough University, Leicestershire, LE11 3TU, UK

Based on classical density functional theory (DFT), we investigate the demixing phase transition of a two-dimensional, binary Heisenberg fluid mixture [1]. The particles in the mixture are modeled as Gaussian soft spheres, where one component is characterized by an additional classical spin-spin interaction of Heisenberg type. Within the DFT we treat the particle interactions using a mean-field approximation. For certain magnetic coupling strengths, we calculate phase diagrams in the density-concentration plane. For sufficiently large coupling strengths and densities, we find a demixing phase transition driven by the ferromagnetic interactions of the magnetic species showing a complex behaviour of the particles similar as in [2]. We also provide a microscopic description (i.e., density profiles) of the resulting non-magnetic/magnetic fluid-fluid interface. Finally, we investigate the phase separation using dynamical density functional theory (DDFT) [3], considering both nucleation processes and spinodal demixing.
[1] K. Lichtner, A. J. Archer, S. H. L. Klapp, J. Chem. Phys., accepted.
[2] R. Rungsawang et al., Phys. Rev. Lett. 104 (2010) 255703.
[3] A. J. Archer and R. Evans, J. Chem. Phys. 121 (2004) 4246.

CPP 10.9 Tue 12:00 C 130

Homogeneous and patterned deposition from a meniscus of an evaporating suspension onto a moving substrate — •Hender Lopez and Uwe Thiele — Department of Mathematical Sciences, Loughborough University, Leicestershire LE11 3TU, UK

A dynamical model is used to study the deposition process observed when an inclined plate is drawn from a bath of a volatile solution or suspension. Based on the gradient dynamics formulation proposed by Thiele [*Eur. Phys. J. Special Topics* 197, 213 (2011)] we derived two coupled equations that describe the film height profile and mean solute concentration. These equations were solved numerically for a large parameter set and the effect of the plate velocity, U, was studied systematically. Our model captures the two main regimens that have been observed in a wide range of experimental setup): at low U, the deposit thickness decreases with U (evaporative regime), and at high U, the deposit thickness increases with U (Landau-Levich regime). An important feature is that for a range of U in the evaporative regime we observe a stick-slip motion of the contact line that is related to the formation of regular lines deposits. This phenomenon is frequently reported in experiments, but often not covered by previous models. We acknowledge support by the EU (PITN-GA-2008-214919).

CPP 10.10 Tue 12:15 C 130

Water interfaces from first principles: structure and spectroscopy — •Marialore Sulpizi — Johannes Gutenberg University Mainz, Staudinger Weg 7 55099 Mainz Germany.

Complex phenomena arise at solid-liquid interfaces, leading to surface induced changes that are not only important for the solid but also for the liquid. In that respect, water plays an important role in a number of interfacial phenomena encountered in biological, chemical and physical processes. Water properties at the interface can be quite different with respect to bulk properties and have been subject of recent research efforts. Here we present some simulation results on solid/water, namely quartz/water and alumina/water, and water/vapor interfaces based on Density Functional Theory. We aim to address the molecular details of the solvation structure and to include the electronic polarization effects. We calculate the acidity of oxide surfaces and we discuss the water structure at the interface to interpret recent experimental results from surface sensitive Sum Frequency Generation.

CPP 10.11 Tue 12:30 C 130

Second Generation Car-Parrinello Molecular Dynamics: Theory and Application to the Liquid/Vapor Interface — •Thomas Kühne — Johannes Gutenberg University Mainz, Institute of Physical Chemistry and Center for Computational Sciences, Staudinger Weg 9, D-55128 Mainz, Germany

A new method [1] to accelerate density functional theory-based ab-initio molecular dynamics simulations is presented. In the spirit of the Car-Parrinello [2] approach during the dynamics the electronic wavefunctions are not self-consistently optimized. However, in contrast to the original scheme, large integration time steps can be used. By this means the best of the Born-Oppenheimer and the Car-Parrinello methods are unified, which not only extends the scope of either approach, but allows for ab-initio simulations previously thought not feasible. The effectiveness of this new approach is demonstrated on liquid water at ambient conditions [3], and on the corresponding liquid/vapor interface [4].

[1] T. D. Kühne, M. Krack, F. Mohamed and M. Parrinello, Phys. Rev. Lett. 98, 066401 (2007). [2] R. Car and M. Parrinello, Phys. Rev. Lett. 55, 2471 (1985). [3] T. D. Kühne, M. Krack and M. Parrinello, J. Chem. Theory Comput. 5, 235 (2009). [4] T. D. Kühne, T. A. Pascal, E. Kaxiras and Y. Jung, J. Phys. Chem. Lett. 2, 105 (2011).

CPP 10.12 Tue 12:45 C 130

The mesoscopic structure of liquid–vapour interfaces — •Felix Höfling and Siegfried Dietrich — Max-Planck-Institut für Intelligente Systeme, Heisenbergstraße 3, 70569 Stuttgart, and Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

The interfacial region between coexisting phases, e.g., between liquid and vapour, is broadened and roughened by thermal fluctuations. The spectrum of these fluctuations diverges for large wavelengths according to capillary wave theory; deviations have been predicted by density functional theory for inhomogeneous fluids [1]. In particular, an enhancement of fluctuations at mesoscopic wavenumbers is expected due to the long-ranged nature of the intermolecular dispersion forces. These predictions have been supported by scattering experiments, but previous computer simulations find a monotone spectrum.

We have performed extensive simulations for a simple liquid with Lennard–Jones interactions truncated at long distance. The investigation of large system sizes was considerably accelerated by a specifically developed simulation package employing high-end graphics processors [2]. Introducing an interfacial structure factor, the wavenumber-dependent surface tension is derived. It develops a maximum at mesoscopic scales as temperature is increased, indicating a relative suppression of fluctuations. We argue that the expected minimum may be masked by the emerging maximum.

[1] K. Mecke and S. Dietrich, Phys. Rev. E **59**, 6766 (1999).

[2] P. Colberg and F. Höfling, Comp. Phys. Comm. **182**, 1120 (2011).

CPP 11: New Instruments and Methods

Time: Tuesday 9:30–13:00 Location: C 243

Topical Talk CPP 11.1 Tue 9:30 C 243

Employing natural search strategies for complex optimization problems — Christoph Schiffmann and •Daniel Sebastiani — Freie Universität Berlin

The Artificial Bee Colony algorithm[1] is a stochastic optimization scheme that mimics the foraging behavior of honey bees. As one of the most recently developed "nature-inspired" algorithms, this approach has turned out to perform very efficiently in global optimization problems from engineering and computer science.

We apply the Artificial Bee Colony algorithm to optimization problems[2] in chemical physics, specifically within ab-initio electronic structure theory. This field is a case in point for highly corrugated potential surfaces which render deterministic approaches unfeasible.

[1] Karaboga, D. & Basturk, B. *J. Glob. Optim.*, **2007**, 39(3), 459–471.
[2] Schiffmann, C. & Sebastiani, D. *J. Chem. Theory Comput.*, **2011**, 7(5), 1307–1315.

CPP 11.2 Tue 10:00 C 243

Excitation Energy Transfer and Optical Properties of Supramolecular Complexes: A Mixed Quantum Classical Methodology — •Jörg Megow[1], Alexander Kulesza[2], Beate Röder[1], Roland Mitric[2], and Volkhard May[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Germany — [2]Institut für Physik, Freie Universität Berlin, Germany

Excitation energy transfer and optical properties of large chromophore complexes are studied using a mixed quantum classical methodology. The chromophore complex is formed by a butanediamine dendrimer to which sixteen pheophorbide-a (Pheo) molecules are covalently linked (P16). While the nuclear coordinates are described classically by carrying out room-temperature MD-simulations the electronic excitations are treated quantum mechanically by solving the time-dependent Schrödinger equation. The energy gap fluctuation due to intramolecular vibration was calculated utilizing a harmonic approximation. The solute-solvent coupling is treated by Coulomb interaction.

Using the energy gap fluctuation, linear absorbance and pump-probe-spectra of P16 are calculated and compared to earlier results calculated for a single Pheo [1] and P4 [2,3]. The effect of the excitonic coupling between the chromophores in P16 was analized in comparison with the results for a single Pheo and P4.

[1] J. Megow et al., Chem. Phys. 377, 10 (2010)
[2] J. Megow et al., ChemPhysChem 12, 645 (2011)
[3] J. Megow et al., Chem. Phys. Lett. (in press)

CPP 11.3 Tue 10:15 C 243

A numerical approach to macroscopic nuclear spin-lattice relaxation by paramagnetic impurities — •Simon Quittek, Michael Ditter, and Franz Fujara — Institut für Festkörperphysik, TU Darmstadt

The influence of paramagnetic impurities on the nuclear spin-lattice relaxation rate has been known for about fifty years. Good heat contact between both systems favors a relaxation path from the nuclei via the impurities into the lattice, which considerably speeds up the bulk relaxation.

Whereas microscopic theory is well investigated, we lack a detailed understanding of the macroscopic processes. Recent field-cycling NMR data reveil a field dependence of the relaxation rate that is not comprised by conventional methods.

To shed some light onto this up-to-date problem, a computer simulation has been performed. The combined relaxation-diffusion equation is solved *ab initio* in a deterministic numeric scheme, which discretizes the considered space. An alternative approach maps the diffusion component onto random walkers, which in turn carry magnetization that is gradually lost when approaching an impurity.

The calculations yield relaxation behaviour that is in good agreement with experimental data. Impurity distributions and magnetic fields are reflected in the field dependent relaxation rates.

CPP 11.4 Tue 10:30 C 243

Temperature modulated optical refractometry: a novel access to structural changes in isotropic media coupling to the optical refractive index — •Ulrich Müller[1], Martine Philipp[2], Roland Sanctuary[1], Peter Müller-Buschbaum[2], and Jan-Kristian Krüger[1] — [1]Université du Luxembourg, Laboratoire de physique des matériaux avancés, , 162a av. de la faiencerie, Luxembourg, Luxembourg — [2]TU München, LS Funktionelle Materialien, Garching, Germany

Temperature modulated optical refractometry (TMOR) is a novel technique that provides access to the dynamic thermo-optic coefficient $\phi^*(\omega) = \frac{1}{n}\frac{dn}{dT}(\omega)$. Similar to temperature modulated calorimetry small sinusoidal temperature perturbations are applied to the sample and their effect on its refractive index n is measured. By applying linear response theory the usually complex susceptibility $\phi^*(\omega)$ is obtained. Simultaneously, the mean refractive index yields information about kinetically induced structural changes. Using the Lorenz-Lorentz equation to relate the refractive index to the mass density the complex coefficient of thermal expansion $\alpha^*(\omega)$ can be calculated out of n and $\phi^*(\omega)$. This novel technique is especially suited for the investigation of (isothermal) structure-changing processes like polymerization, solvent evaporation, and isostructural phase transitions (e.g. glass transitions or volume phase transitions), where it allows for an easy discrimination of kinetic and dynamic contributions. Investigations of the chemically induced glass transition in an epoxy and of the volume phase transition in PNIPAM/water are presented as applications.

CPP 11.5 Tue 10:45 C 243

Infrared Transition Moment Orientational Analysis on semicrystalline polyethylene films — •Wilhelm Kossack[1], Periklis Papadopoulos[2], Matthew Parkinson[3], Floran Prades[3], and Friedrich Kremer[1] — [1]Universität Leipzig, Linnéstrasse 5, 04103 Leipzig, Germany — [2]Max Planck Institute for Polymer Research, Postfach 3148, 55021 Mainz, Germany — [3]Borealis Polyolefine GmbH, St.-Peter-Strasse 25, 4021 Linz, Austria

The recently developed method of Infrared-Transition-Moment-Orientational-Analysis (IR-TMOA) is based on concurrent measurements of the transmission in dependence on polarisation of the IR light and on the inclination of the sample with respect to the optical axis. This enables one to determine for the different molecular moieties of the studied material the full order parameter tensor and its orientation with respect to the sample coordinate system. The analysed films, made by a blown film process, show only low ordered crystalline regions (order parameters <0.3) and an even less ordered amorphous matrix (Kossack, et al., doi:10.1016/j.polymer.2011.10.051). The method provides a quantitative insight into the correlation of production parameters and microscopic structure playing a key role to improve the properties of polyolefin fims.

CPP 11.6 Tue 11:00 C 243

Characterization of morphology and orientation of uni-axially oriented cast films with confocal and polarized μ-Raman Imaging-Spectroscopy — •Krisztina Vincze-Minya, Tobias Keplinger, and Sabine Hild — Institute of Polymer Science, Johannes Kepler University, Altenbergerstr. 69, 4040 Linz, Austria

The morphology of a semi-crystalline polymer has a great bearing on its mechanical strength. The ratio of crystalline and amorphous phases and molecular orientation in these phases are essential to optimize the physical properties. Confocal μ-Raman microscopy is a useful characterization technique to characterize the orientation not only of the crystalline but also of the amorphous phase. With confocal μ-Raman Imaging it is possible to calculate not only an average crystallinity, but also to determine the local crystallinity. The main focus is to calculate the crystallinity degree and to characterize the orientation of the uni-axially oriented PP cast films. The ratio of the peaks at 841 and 809 cm-1 is sensitive to the molecular anisotropy and the crystallinity values were calculated by the Nielsen method[1]. The ratios I(809)/I(841) and I(973)/I(998) are used for the characterization of orientation heterogeneity (I = intensity of a peak)[2]. Based on these results the orientation and crystallinity of shear crystallized samples are investigated. [1]Nielsen A.S., Batchelder D.N., Pyrz R ,2002, Polymer, 43(9), 2671-2676 [2]J. Martin, S. Margueron, M. Fontana, M. Cochez, P. Bourson, 2009, Polymer Engineering & Science, 50(1), 138-143

15 min break

CPP 11.7 Tue 11:30 C 243

Twin-Focus Photothermal Correlation Spectroscopy — •Markus Selmke, Marco Braun, Romy Schachoff, and Frank Cichos — Universität Leipzig, Exp. Physik I, molecular nanophotonics

The use of metal nano-particles for probing dynamics and reactions in biology and soft-matter physics has been on the rise due to their superior stability as compared to molecular fluorophores. The successful method of fluorescence correlation spectroscopy (FCS), which quantifies in its simplest form locally the diffusion and mobilities, has found its counterpart for these non-fluorescent but absorbing nano-tracers in PhoCS, photothermal correlation spectroscopy. The signal used in this method for the detection is related to the plasmonic heating of the particles: The power absorbed from a resonant laser (532nm) generates a temperature profile around the particle which in turn causes a refractive index profile which is probed by a second off-resonance laser, typically by means of a lock-in technique. While the lensing action provides a twin-focus split detection-volume in which two non-overlapping regions may be addressed and analyzed individually or in combination it is also clear that the absorption infers momentum to the diffusing particles which may be addressed and studied by the advection-diffusion equation and its effect on various (cross-)correlation functions. These features allow for the sensitive determination of minute flow velocities, either self-induced by radiation pressure or via external forces, and the study of heterogeneous dynamics on the length scale of the split-focus separation (about 500nm).

CPP 11.8 Tue 11:45 C 243

Organic reactions at ionic liquid surfaces studied by in-situ XPS — •Inga Niedermaier[1], Claudia Kolbeck[1], Nicola Taccardi[2], Peter Schulz[2], Peter Wasserscheid[2], Hans-Peter Steinrück[1], and Florian Maier[1] — [1]Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen — [2]Lehrstuhl für Chemische Reaktionstechnik, Egerlandstr. 3, 91058 Erlangen

Due to their low vapour pressure, ionic liquids - organic salts with a melting point below 100 °C - can be investigated by surface science techniques under UHV conditions. In particular, angle-resolved X-ray photoelectron spectroscopy (ARXPS) has been proven to be an effective tool for studying molecular enrichment and orientation effects even for the topmost surface layers of the ionic liquid. Here, we demonstrate that ARXPS also allows accessing classical organic chemical reactions normally carried out in common solvents, by employing reactive centres covalently fixed to cations or anions of ILs. This novel concept is successfully carried out for a nucleophilic substitution where a tertiary amine attached to an imidazolium cation is alkylated by the chloroalkyl moiety of the anion. In course of the reaction, covalently bound chlorine (neutral) is converted to chloride (negatively charged) and amine (neutral) to ammonium (positively charged). These changes are reflected by characteristic shifts in the N 1s and Cl 2p ARXP spectra. In this respect, in-situ ARXPS represents a novel tool to analyse reaction pathways at liquid surfaces on a molecular level. - Supported by the DFG through SPP 1191 and by the Cluster of Excellence - Engineering of Advanced Materials.

CPP 11.9 Tue 12:00 C 243

Piezoelectric PVDF as an acoustically calibrated transducer — •Marcel Kappel, Gunnar Gidion, and Reimund Gerhard — Universität Potsdam, Institut für Physik und Astronomie, Potsdam

The application of piezoelectric polyvinylidene fluoride (PVDF) as a calibrated acoustical sensor is tested and characterized with different methods. Characteristic parameters, such as the static pressure and the amplitude of the dynamical force on the PVDF film, as well as the sensor long term stability, are varied in order to evaluate the effectivity and durability of the electro-mechanical conversion represented by the piezoelectric coefficient d_{33}. Also the frequency response of the piezopolymer as sensor and actuator was investigated. Using thin film sensors made from PVDF, we describe measurements made on a conceptional piano model and on a real piano manufactured by Bechstein. The PVDF probes were mounted between the resonance board and the sound bridge, in combination with a condensor microphone for airborne sound. Beside both recording techniques were directly compared, the temporal distribution of the vibrational energy within the measured setup could be deduced.

CPP 11.10 Tue 12:15 C 243

Soft colloidal probe AFM for quantifying mechanoresponsive brushes — •Johann Erath[1], Johanna Bünsow[2], Wilhelm T. S. Huck[2,3], and Andreas Fery[1] — [1]Physical Chemistry II, University Bayreuth, Universitätsstraße 30, 95440, Bayreuth, Germany — [2]Melville Laboratory for Polymer Synthesis, Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB21EW, UK — [3]Radboud University Nijmegen, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands

The aim of this contribution is to introduce a novel concept for self-reporting force sensors based on mechano-responsive polyelectrolyte brushes, which translate deformation and tension directly into changes of fluorescence intensity[1]. Force sensing experiments were performed with a combination of an atomic force microscope (AFM) with a confocal laser scanning microscope (CLSM), using the soft colloidal probe (SCP) technique. On the basis of the JKR theory, we developed a quantitative understanding of the force distribution underneath the PDMS bead, which shows that the sensor does response to compression and tension. We find an excellent pressure sensitivity in the order of 1 kPa and a lateral resolution better than 1 micron. Beside the basic concept of the technique we will show perspectives for mapping pressure fields.

[1] Bünsow, J.; Erath, J.; Biesheuvel, M.; Fery, A.; Huck, W. T. S., Angewandte Chem. Int. Ed., 50, (2011) 9629-9632 Highlighted by Nature Materials 2011, 10, p. 724

CPP 11.11 Tue 12:30 C 243

Application of novel thermal cantilever in the field of polymer science — •Thomas Fischinger, Martin Laher, Günther Gratzl, and Sabine Hild — Department of Polymer Sciences, Johannes Kepler University, Linz, Austria

Thermal analysis methods are generally used to provide important and reliable data on polymeric materials. However, up to now mainly bulk properties of polymers have been detected. Their fields of operation reach a limit for applications such as investigation of thin films, immiscible polymer blends, boundary effects etc. Therefore, a method is proposed for nano-thermal characterization of polymers using scanning probe microscopy in combination with heatable cantilever probes. This method is based on an appropriate temperature calibration, which provides a reliable correlation between applied voltage and the temperature at the tip. Since it has been shown that the presented technique is substantially more susceptible to environmental changes, such as layer thickness, substrate material etc. than comparable macroscopic approaches, parameters that might influence the performance have been evaluated. To verify the validity and show the possibilities of this method, local thermal analysis measurements were performed on different polymer samples. The glass transition- and melting temperature obtained by our approach agrees well with the value measured using conventional bulk methods.

CPP 11.12 Tue 12:45 C 243

Bimetallic cantilever microcalorimetry with high energy and time resolution — •Florian M. Spirkl, Richard Schröter, Friedrich Esch, and Uli Heiz — TU München, Lehrstuhl f. Physikalische Chemie

Temperature induced bending of bimetallic cantilevers has been established in recent years as sensor for microcalorimetry, offering high energy resolution [1]. The position of the cantilever tip is read out using a laser and a position sensitive optical device (PSD). We present a differential read out setup that improves the time resolution from typical 100 ms [2] down to 1 ms, the response time of the cantilevers that is time-limiting.

The experimental setup consists of a reactive sample and an inert reference cantilever that are read out differentially using a high frequency deflection mirror. Both bend simultaneously due to environment changes, whereas the investigated process develops heat only on the sample cantilever. For calibration, both sample and reference cantilever can be heated by two laser diodes. This cantilever setup works under UHV conditions, and in reactive gas as well as in liquid environment. The sensitivity of the ambient cantilever setup can be estimated to be 150 nJ with 1 ms time resolution.

First experiments within a temperature controlled liquid flow cell will be presented, including measurements on thiol-gold bonding upon formation of self-assembled monolayers (SAM).

[1] J.R. Barnes *et. al.*, *Review of Scientific Instruments* **65**, 3793, (1994) [2] H.P. Lang *et. al.*, Materials Today **8**, 30 (2005)

CPP 12: Glasses II (joint session with DY)

Time: Tuesday 10:00–12:30 Location: MA 004

CPP 12.1 Tue 10:00 MA 004

The coupled energy landscape model — •Christian Rehwald and Andreas Heuer — Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, 48149Münster

While the dynamics of small glass-forming systems can be described by properties of the underlying potential energy landscape (PEL), this concept breaks down in large systems. Here we present the “coupled energy landscape model” (CLM) which extends the PEL description to macroscopic system by introducing a coupling mechanism between the PEL of elementary systems (ES).

First we use the distance dependence of structural relaxations after an initial reorganization in an iso-configurational ensemble of a non-equilibrium configuration. The results indicate the existence of a causal connection between successive events, which can be identified as dynamical coupling between ES.

In a next step we use different observables to extract coupling mechanisms and their strength in the CLM from MD simulations (of a binary mixture of LJ particles): Finite size effects of τ_α and the non-exponentiality parameter β_{KWW} are proving to be an appropriate measure for comparing the two dynamics. The CLM combines advantages of recently discussed models for the glass transition like facilitated spin models and the mosaic approach and can be used to understand principles of glassy dynamics like increasing τ_α and emergence of the growing dynamical length scale χ_4.

CPP 12.2 Tue 10:15 MA 004

Glassy dynamics on the atomic scale measured with XPCS — •Manuel Ross[1], Michael Leitner[1,2], Markus Stana[1], and Bogdan Sepiol[1] — [1]Department of Physics, University of Vienna, 1090 Vienna, Austria — [2]Physics Department E13, Technical University of Munich, 85747 Garching, Germany

The world of solids can be divided into crystals and amorphous materials. One of physics’ unsettled questions is the dynamic behavior of these amorphous materials, especially that of glasses. In our group, we developed a new method for observing dynamics on the atomic level [1]. Utilizing the most brilliant X-rays generated by high energy synchrotron sources and measuring in the diffuse regime of scattering, the principle of photon correlation spectroscopy can be extended to the sub-nanometer range. We currently apply our method to glasses in order to shed light on the processes which govern glassy dynamics. In particular, we study lead and silicate glasses, where the network is built of tetrahedral structures. I will present our recent results obtained from measurements at ESRF and PETRA III and the consequences for our view on the atomic dynamics of glasses.

[1] M. Leitner, B. Sepiol, L. M. Stadler, B. Pfau, and G. Vogl, Atomic diffusion studied with coherent X-rays, Nature Mat. 8, 717 (2009).

CPP 12.3 Tue 10:30 MA 004

Computer simulation of micro-rheology in glass-forming systems — David Winter[1] and •Juergen Horbach[2] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany — [2]Institut für Theoretische Physik II, Heinrich Heine-Universität Düsseldorf, Universitätsstr. 1, 40225 Düsseldorf, Germany

In the last ten years, micro-rheology has been established as a new tool to probe the non-linear response of soft-matter systems to external fields. In a micro-rheological experiment,single particles are pulled through a viscous medium by a constant or oscillatory force using, e.g., optical tweezers. In the work presented in this talk, the single-particle response to a constant external force of varying strength is investigated for a glass-forming Yukawa mixture using molecular dynamics computer simulation. Beyond linear response, a scaling regime is found where a force-temperature superposition principle of a Peclet number holds. In the latter regime, the diffusion dynamics perpendicular to the force can be mapped on the equilibrium dynamics in terms of an effective temperature whereas the diffusion coefficient parallel to the force does not exist. This behavior is associated with a hopping motion of the pulled particle from cage to cage and can be qualitatively understood by a simple trap model, as proposed by Bouchaud and coworkers.

CPP 12.4 Tue 10:45 MA 004

Statistical analysis of the non-linear dynamics of a supercooled model fluid under a microrheological perturbation — •Carsten Schroer[1,2] and Andreas Heuer[1,2] — [1]Institut für physikalische Chemie, Münster, Germany — [2]Graduate School of Chemistry, Münster, Germany

In our approach we regard the complex dynamics of glass-forming systems as a stochastic process on the potential energy landscape (PEL). Via computer simulations it is possible to map the continuous dynamics onto a hopping motion between the corresponding inherent structures of the system. We find mesoscopic regions (metabasins) in the PEL where the system is located for long times so that dynamics is mainly determined by the transitions between those metabasins. These discrete processes allow us to describe the dynamics in terms of a continuous time random walk.

This approach is of particular interest when including a microrheological perturbation via non-equilibrium molecular dynamic simulations. We report how linear and non-linear responses translate into the continuous time random walk properties of the system. Furthermore we show what consequences for the pathway of the system in its PEL arise by the application of a microrheological perturbation. We discuss these effects in terms of a rejuvenation scenario.

CPP 12.5 Tue 11:00 MA 004

Glass structure with well defined thermal history and glassy dynamic — •Christoph Scherer[1,2], Friederike Schmid[1], and Martin Letz[2] — [1]Institut fuer Physik, Johannes-Gutenberg Univ. Mainz, Staudingerweg 9, 55099 Mainz — [2]Schott AG, Hattenbergstr. 10, 55122 Mainz

Glasses have a huge range of applications, however, they are still theoretically not well understood. Also experimental access to the structure of glasses is limited. This motivates the study of glass systems by means of computer simulations. In this work a set of glass structures with well defined thermal history is generated on the computer. Each glass structure is created by gradually cooling down a set of 100-200 atoms by means of a molecular dynamics simulation as long as the system still can be equilibrated in reasonable simulation time. Afterwards, it is quenched down to room temperature and the resulting atom coordinates and velocities are stored. They are used as a starting point for a quantum-mechanical relaxation by means of density functional theory. Then the vibrational spectrum is determined and compared to experimental results. From the vibrational spectrum a set of thermodynamic quantities, as the temperature dependent specific heat, are obtained and compared to measured data. First successful tests on the model glass former SiO2 are presented.

CPP 12.6 Tue 11:15 MA 004

Microscopic picture of the beta-wing in simulated Ni0.5Zr0.5 melt — •Helmar Teichler — Inst. f. Materialphysik, Univ. Göttingen, Göttingen, Germany

The beta-wing is found in a large variety of liquids as an additional contribution to the susceptibility on the high frequency flank of the alpha peak. The underlying microscopic processes are not well understood so far. Regarding this, we have analyzed simulation data of a Ni0.5Zr0.5 model, using as main tool the fraction of un-displaced particles (FUDP). In the alpha and beta regime, the FUDP is a nearly linear mapping of the incoherent intermediate scattering function (ISF) (for suitably q) (H. Teichler, PRL, 107,067801 (2011)). Hence, the susceptibilities of FUDP and ISF display nearly identical alpha peak and beta-wing. The analysis unambiguously shows that this susceptibility is due to temporal accumulation of incoherent short-ranged displacement processes, where the stretched exponential behavior reflects ”structure conserving correlations” in the accumulation process. Accordingly, the beta-wing reflects stronger structure restoring effects in the wing range than in the rest of the alpha regime.

CPP 12.7 Tue 11:30 MA 004

Glass form factors in confined geometry — •Simon Lang[1], Vitalie Botan[2], Martin Oettel[2], Rolf Schilling[2], and Thomas Franosch[1] — [1]Friedrich-Alexander Universität, Erlangen, Germany — [2]Johannes Gutenberg-Universität, Mainz, Germany

Supercooled liquids embedded in complex geometries exhibit an intriguing interplay between particle interaction and incommensurability

effects. Recently, the mode-coupling theory (MCT) of the glass transition was elaborated for a symmetric hard-wall confinement, where the glass-transition line reveals a striking re-entry phenomenon by varying the wall-to-wall separation [1]. A subtle point of the mathematical structure of these MCT equations is the emergence of two relaxation channels, which arise from a splitting of the current into a parallel and perpendicular direction with respect to the walls. Here, we present the glass form factors evaluated at the critical point for several distances. These arrested parts of the intermediate scattering function yield information about the structural arrangement of the particles in the confined glass state. We show, that the structure changes drastically upon varying the wall separation and the hallmarks of the phase diagram for confined liquids are reflected in the glass form factor. We demonstrate that the MCT equations for the glass form factor in confinement can be solved by a convergent iteration. From a generalized covariance property, the maximum principle for the glass form factors holds also for the MCT for confined liquids.
[1] S. Lang, V. Boţan, M. Oettel, D. Hajnal, T. Franosch, and R. Schilling, Phys. Rev. Lett.105 125701 (2010).

CPP 12.8 Tue 11:45 MA 004

Transient stresses and MSDs in sheared dispersions as described by mode-coupling theory (MCT) — •Christian Peter Amann and Matthias Fuchs — Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

Sheared viscoelastic media exhibit a stress overshoot between elastic and plastic regime, i.e. a maximum in the shear stress vs strain plot after switching on a constant shear rate. This maximum characterizes the transient evolution between equilibrium and steady state. A way to model such overshoots is the $F_{12}^{(\dot\gamma)}$ model, a schematic model in MCT to describe glass forming liquids. This approach is tested by comparing results with various rheological experiments. Flow curves, linear- and non-linear stress response, and stress-strain curves can be fitted consistently with the same model [1,2]. Within microscopic MCT the stress overshoot is identified as negative dip in the dynamic stress autocorrelation function [3].

This mechanism also causes super-diffusive colloid motion [3]. We connect shear stress and colloidal MSD via a generalized Stokes–Einstein relation and compare shear–stress and MSD simulations to define a characteristic strain determining maximum shear stress and onset of superdiffusion.

[1] M. Siebenbürger et al., *J. Rheol.* **53**, 707–726 (2009)
[2] J.M. Brader et al., *Phys. Rev. E* **82**, 061401 (2010)
[3] J. Zausch et al., *J. Phys.: Condens. Matter* **20**, 404210 (2008)

CPP 12.9 Tue 12:00 MA 004

Probing Spectral Diffusion Theory in Glasses Through Polarization Echo Measurements — •Gudrun Fickenscher, Christian Schötz, Paul Fassl, Masoomeh Bazrafshan, Manfred von Schickfus, Andreas Fleischmann, and Christian Enss — Kirchhoff Institute, Heidelberg University, Germany

Many low temperature properties of glasses can be well described by the standard tunnelling model. It assumes an ensemble of isolated tunnelling systems (TS) with a broad distribution in energy splitting and asymmetry. They can couple resonantly to electric fields and can therefore be probed by polarization echo measurements. When looking at dynamic properties of glasses, however, the influence of the TSs in the surrounding of the resonantly probed TSs has to be taken into account. Spectral diffusion theory* assumes that transitions in thermally excited TSs change the local fields at the positions of the resonant TSs, thus changing their energy splitting and phase. This affects the decay behaviour of the polarization echo amplitude with respect to the delay time.

We have performed different types of polarization echo measurements including 2-pulse echoes which show an almost pure T_2 decay and 3-pulse echoes which are more sensitive to T_1 processes. The setup allows for measurements with very long delay times of several milliseconds. We calculated the decay in echo amplitude within the framework of the spectral diffusion theory and compared the results.

* J.L. Black, B.I. Halperin, Phys. Rev. B **16** (1977), 2879.

CPP 12.10 Tue 12:15 MA 004

Dielectric polarization noise and permittivity - A fluctuation-dissipation analysis during the curing of an epoxy resin — Clemens Hassel, •Andreas Reiser, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg

Dielectric spectroscopy as a driven method combined with non-driven dielectric noise spectroscopy is a powerful experimental method for studying the fluctuation-dissipation theorem experimentally. We apply both methods during the curing process of the epoxy resin Epon 828 with n-butylamine. Setting the sample temperature properly allows controlling the time scale of curing. We measure in the temperature range between 293 K and 303 K at fixed temperatures. During curing the Epon-n-butylamine mixture undergoes a chemically induced glass transition. We analyze the validity of the fluctuation-dissipation theorem and calculate an effective temperature for this system.

CPP 13: Poster: Interfaces and Thin Films

Time: Tuesday 18:15–20:45 Location: Poster A

CPP 13.1 Tue 18:15 Poster A

Critical Adsorption of Polymers with Different Architecture — •Olga Mironova[1] and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e. V., Dresden, Germany — [2]TUD, Dresden, Germany

In order to understand the role of the chain architecture for the adsorption properties of polymers, we simulate polymer systems using the bond-fluctuation model (BFM). End-grafted polymers at an adsorbing surface are considered under good solvent conditions and we analyzed our results using scaling arguments. Suggestion, that adsorption properties of polymers, such as critical energy of adsorption and crossover exponent, for instance, can differ between molecules with the same molecular weight, but with different architectures, can be used as basis in separation technique (Liquid chromatography at the critical condition-mass spectrometry) of such molecules. We consider molecules with three different types of architecture: linear, star-shaped and hyperbranched. It was found that critical parameters for 4-arms star-shaped polymers and linear chains are very close to each other. To determine the critical parameters for hyperbranched polymers ensemble averages over many realizations of the branching topology is necessary. Variations of the branching probability gives access to experiments on hyperbranched polymers.

CPP 13.2 Tue 18:15 Poster A

Influence of charge density on bilayer bending rigidity in lipid vesicles: a combined dynamic light scattering and neutron spin-echo study — •Beate-Annette Brüning[1], Ralf Stehle[1,2], Peter Falus[3], and Bela Farago[3] — [1]Helmholtz Zentrum Berlin, Hahn-Meitner Platz 1, 14109 Berlin, Germany — [2]Universität Bayreuth, Postfach 10 12 51, 95440 Bayreuth, Germany — [3]Institut Laue-Langevin, B.P. 156, 6 rue Jules Horowitz, 38042 Grenoble, France

We report a combined dynamic light scattering and neutron spin-echo study on vesicles composed of the uncharged helper lipid DMPC and the cationic lipid DOTAP. Mechanical properties of a model membrane and the corresponding fluctuation dynamics can be tuned by changing composition. We compare the bilayer undulation dynamics in lipid vesicles composed of DMPC/DOTAP to vesicles composed of DMPC and the also uncharged reference lipid DOPC. We find, that on the local scale, lipid headgroup composition and charge change the vesicle fluctuations less than acyl chain packing inhomogenities between the composite lipids. We discuss this result on the basis of domain formation in the lipid mixtures containing charged (DMPC/DOTAP) and uncharged reference lipid (DMPC/DOPC). First, we investigate lipid vesicle size and mass diffusion using dynamic light scattering, then we study collective bilayer undulations and bulk diffusion on two distinct time scales around 25ns and 150ns, using neutron spin-echo spectroscopy. Finally, we estimate bilayer bending rigidities κ_B for the charged and uncharged lipid vesicles.

CPP 13.3 Tue 18:15 Poster A

Monte-Carlo Simulation of Compatibilization by Network-

Building and Catalytic Interface Reactions in Two-Component Injection Molding — •Andreas John, Jürgen Nagel, and Gert Heinrich — Leibniz Institut für Polymerforschung Dresden e. V., Hohe Strasse 6, 01069 Dresden

Adhesion of immiscible polymers during two-component injection molding can be improved by transreactions of properly functionalized molecules in situ by exploitation of the thermal energy of the melts.To investigate these processes, we performed Monte-Carlo (MC) simulations based on the three-dimensional coarse-grained Bond Fluctuation Model (BFM) including a thermal interaction potential in r<=sqrt(6) with energy eps=0.1kBT. We compared a simple Split type reaction, which is capable of network-forming, with a catalytic interface reactive process both exhibiting different values of activation energy. The main process of the catalytic reaction system is identical to the simple Split reaction as described previously, but now a reactive monomer creating process is prefixed. For the reacting systems different physical properties like consumption, radius of gyration, concentration profiles or the distribution of the degree of polymerization were calculated as a function of time. Additionally, several functions for the description of the adhesive strength on the molecular level were adopted and calculated depending on reaction type, activation energy and degree of consumption, respectively. From the results, those chemical reaction types were deduced, which should be most suitable for compatibilization intentions in two-component injection molding.

CPP 13.4 Tue 18:15 Poster A

Molecular Dynamics of Miscible Polymer Blend Thin Films — •Huajie Yin and Andreas Schönhals — BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany

Molecular dynamics of Polystyrene (PS), Poly(vinyl methyl ether) (PVME) and their blend (PS/PVME) confined in thin film geometry have been studied by mean of broadband dielectric spectroscopy (BDS). No thickness dependence of PS segmental dynamics was observed down to 14 nm. For pure PVME, three relaxation processes (Alpha,Beta and Gamma) were observed. The Arrhenius plots of the Beta and Gamma processes have activation energy of 38.3 kJ/mol and 20.5 kJ/mol, respectively. The relaxation rate of the Alpha process is well described by the Vogel-Fulcher-Tamman (VFT) equation. Thin films of PS/PVME polymer blend in the weight ratio of 25/75 have been investigated for different thicknesses. The broadening of the Alpha-relaxation peak for the polymer blend was observed, the intensity of which increases with the temperatures. The glassy dynamics of the polymer blend thin films are independent of the layer thickness under study.

CPP 13.5 Tue 18:15 Poster A

Implementation of super-structures on mesoporous titania films via soft embossing — •Gregory D. Tainter, Martin A. Niedermeier, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany

Metal oxide thin films are the subject of numerous studies due to their potential as photoactive layers, e.g. in photocatalysis and photovoltaics. Using diblock copolymer scaffolds to control the morphologies of mesoporous titania films has been shown to be effective in improving the specific area of such films. The benefits of super-structuring have been successfully demonstrated in the past. A light trapping effect can lead to enhanced absorption in the film which is a highly desirable property for optoelectronic devices.[1]

In this work, hybrid polymer/titania films are prepared via a sol-gel route. The diblock copolymer poly(styrene - block - ethylene oxide) is used to create a mesoporous titania structure through good-poor solvent induced phase separation. The results of soft embossing such hybrid films with varying pressures and temperatures are investigated using optical microscopy, atomic force microscopy and scanning electron microscopy. The optical properties are probed with UV/Vis spectroscopy.

[1] Niggemann et al., Physica status solidi. A 205 12, 2862 (2008)

CPP 13.6 Tue 18:15 Poster A

Electrodeposition of porous ZnO in the presence of sodium dodecylbenzene sulfonate (NaDBS) as structure-directing agent — •Magnus Schäfer, Max Beu, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

ZnO was electrodeposited on fluorine-doped tin oxide (FTO) on glass using an aqueous $ZnCl_2$-solution as electrolyte, heated up to 70°C. A constant voltage of $-1060mV$ vs. a $Ag/AgCl$ reference electrode was used for the deposition. To form a porous ZnO-layer, $sodiumdodecylbenzenesulfonate(NaDBS)$ was added as structure-directing agent to the electrolyte. After the deposition the $NaDBS$ was desorbed from the ZnO electrodes. The influence of $NaDBS$ on the porous structure and on the morphology of ZnO was studied. The subsequent adsorption of organic dyes as sensitizers to the porous zinc oxide layers and their characteristics in dye-sensitized solar cells was tested to analyze the suitability of the porous ZnO matrix as electrode material.

CPP 13.7 Tue 18:15 Poster A

Competing Ordering Processes at Liquid Crystal Surfaces Laden with Semifluorinated Alkane Molecules — •Xunda Feng[1], Ahmed Mourran[2], Martin Möller[2], and Christian Bahr[1] — [1]Max-Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for Technical and Macromolecular Chemistry, RWTH Aachen, Germany

We present an ellipsometric study of the interface between isotropic liquid crystals (LCs) and air in the vicinity of the nematic – isotropic and smectic-A – isotropic transition. The LCs are doped with a small amount of the semifluorinated alkane $C_{18}H_{37}$–$C_{12}F_{25}$ ($H_{18}F_{12}$) which forms a Gibbs film (GF) at the LC/air interface. Our measurements elucidate the interplay between the nematic or smectic surface order at the isotropic LC/air interface and a structural phase transition in a GF on the same interface.

GFs of $H_{18}F_{12}$ on normal alkanes are known to exhibit a transition from a dilute state at higher temperatures to a dense state at lower temperatures. Our results indicate that the same transition takes place in GFs formed on the isotropic LCs. The transition temperature can be tuned by controlling the $H_{18}F_{12}$ concentration in the bulk LC phase. When the transition takes place in the temperature range in which a molecular thin smectic or nematic film exists at the isotropic LC/air interface, the smectic surface order is destroyed while the nematic surface order is affected by a change of the orientation of the LC molecules. The ellipsometric data indicate that both behaviors result from a change of the anchoring condition of the LC molecules in contact with the GF.

CPP 13.8 Tue 18:15 Poster A

Stimuli-responsive layer-by-layer films containing block copolymer micelles — •Inna Dewald[1], Julia Gensel[1], Johann Erath[1], Eva Betthausen[2], Axel H.E. Müller[2], and Andreas Fery[1] — [1]1Physical Chemistry II, University of Bayreuth, 95440, Germany — [2]Macromolecular Chemistry II, University of Bayreuth, 95440, Germany

We report on a novel approach for the design of stimuli-responsive thin films based on the incorporation of charged core-shell-corona micelles consisting of a hydrophobic core, a pH-responsive shell and a permanently charged cationic corona. [1,2] The films were produced using the layer-by-layer technique. Thereby the micelles were electrostatically self-assembled in an alternating manner using a strong anion as binding partner. Our results reveal that the assemblies exhibit fully reversible swelling transition due to pH-response of the weak polyelectrolyte middle block. The swelling behavior shows a strong dependence on solution pH and bilayer number. In order to characterize the multilayer films and analyze their pH-dependent behavior methods such as ellipsometry and atomic force microscopy were used. Measurements for both methods were performed on air as well as in liquid resulting in an up to ten-fold increase of the film thickness compared to the dry thickness. The films capacity of reversible swelling due to changes of solution pH makes our multilayer films excellent candidates for future applications in e.g. drug delivery with controlled release mechanism.

[1] E. Betthausen et al., Soft Matter, 2011, 7, 8880
[2] J. Gensel et al., Soft Matter, 2011, 7, 11144

CPP 13.9 Tue 18:15 Poster A

In Situ Growth Studies of N-Alkanes on Silica with Real-Time X-Ray Methods — •Christopher Weber[1], Christian Frank[2], Wolfram Leitenberger[3], Frank Schreiber[2], and Stefan Kowarik[1] — [1]Institut für Physik, Humboldt Universität zu Berlin, 12489 Berlin — [2]Institut für angewandte Physik, Universität Tübingen, 72076 Tübingen — [3]Institut für Physik, Universität Potsdam, 14476 Potsdam-Golm

We use n-alkanes as a model system to study how the chain-length of molecules influences thin film growth. Because of their insulating properties n-alkanes also have attracted some technological attention. Recently they have been used with great success to improve the performance of an organic field effect transistor. Real-time x-ray methods combined with theoretical models allow us to monitor the growth process in situ, determine changes of the growth modes and follow the roughening of the films. Grazing Incidence X-ray Diffraction allowes to find also some chain-length dependency within the final film structures.

CPP 13.10 Tue 18:15 Poster A

Wetting of solid surfaces by microemulsions — •Stefan Wellert[1], Samantha Micciulla[1], Roland Steitz[2], Regine von Klitzing[1], and Thomas Hellweg[3] — [1]TU Berlin, Str. d. 17. Juni 124, 10623 Berlin, Germany — [2]Helmholtz Center Berlin, Hahn-Meitner Platz 1, 14109 Berlin, Germany — [3]University of Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany

The increasing use of bio-inspired surfactants in microemulsions leads to an increasing interest in these thermodynamically stable self-assembled structures of oil, water and amphiphiles. Although the interaction between such microemulsions and solid surfaces is essential for many desired functionalities, only few is known about local structure and dynamics of a microemulsion in the vicinity of a solid surface. In particular, the influence of surface hydrophobicity, surfactant adsorption, bending elasticity of the amphiphilic interface and related properties have to be investigated in future studies. We used different methods to investigate the interaction of microemulsions with solid surfaces. Measurements of wetting properties at hydrophilic, partially hydrophobic and hydrophobic surfaces were combined with scattering methods resolving the structure of the microemulsion at the various solid surfaces. The resulting structural parameters and the observed dynamics in the vicinity of surfaces are compared to the corresponding results measured in the bulk phase with the undisturbed volume phase structure.

CPP 13.11 Tue 18:15 Poster A

Deformation and Buckling of Elastic Capsules — •Sebastian Knoche and Jan Kierfeld — TU Dortmund

We investigate the deformation behavior of soft elastic capsules. Based on nonlinear shell theory, a theoretical model for liquid filled capsules hanging from a capillary in a pendant drop geometry is developed, and shape equations are derived.

Their deformation behavior upon (a) changing gravity forces (by changing the phase contrast between liquids) and (b) reducing capsule volume is analyzed numerically. In case (a), the capsule stretches and sags and in case (b) we find a rich bifurcation behavior between buckled shapes; the preferred configurations are deduced from a least-energy principle. Based on theoretical results we develop a fitting procedure which allows us to extract the elastic moduli of the capsule membrane from experimental data.

We use similar methods to analyze the buckling behavior of spherical capsules upon reduction of the capsule volume. By preventing self-intersection for strongly reduced volume, we obtain a complete picture of the buckling process and can follow the transition from the undeformed configuration into the fully buckled state.

CPP 13.12 Tue 18:15 Poster A

Microfabrication and characterization of stress-reduced YSZ membranes — •Florian Kuhl, Markus Piechotka, Torsten Henning, Daniel Reppin, Peter J. Klar, and Bruno K. Meyer — I. Physikalisches Institut, Justus Liebig University, Heinrich-Buff-Ring 16, 35392 Giessen

The oxygen conductor YSZ (Yttria-stabilized-zirconia) is a material often used as electrolyte for solid oxide fuell cells. To achieve a higher packing density and to optimize the currents it is necessary to miniaturize the fuel cell components, especially to reduce the thickness of the solid electrolyte. Another application of very thin YSZ films may be their utilization as ion source. Si wafers were locally pre-thinned by photolithography and crystallographic etching to provide pre-thinned areas on which the YSZ thin film was deposited by RF sputtering. Free standing membranes were created by wet chemical etching of the thinned portions of the wafer using a variety of masking patterns defined by electron beam lithography and optimized to reduce stress induced cracking. Since the growth of the YSZ is not completely free of stress, membrane crack issues were observable. We show how the fabrication influences the stress of the sputtered YSZ. For characterization of the fabricated membranes we used light- and laser microscopy as well as SEM and AFM. Additionally, we applied Raman mapping to see how the stress of the YSZ membranes changes the behavior of the Raman modes.

CPP 13.13 Tue 18:15 Poster A

The interplay of structure and molecular dynamics in confinement of block copolymer meso-phases in thin layers — Markus Fuchs, •Martin Tress, Emmanuel Mapesa, and Friedrich Kremer — Universität Leipzig, Leipzig

Broadband Dielectric Spectroscopy (BDS) in combination with X-ray scattering is applied to investigate the molecular dynamics and the meso-phase morphology of the block copolymer system poly(isoprene-b-styrene) confined to thin layers. For the isoprene block, BDS enables one to study the segmental dynamics, taking place on a length scale of ∼0.5 nm, and chain dynamics, which cover length scales of tens of nanometers, separately at the same time. Different compositions of the block copolymer are selected according to their particular meso-phase structure and thin layers are deposited onto recently developed nano-structured electrode arrangements for the BDS measurements. By that, and the complementary structural investigations by X-ray scattering, the interplay of the meso-phase structure and the molecular dynamics on different length scales is examined.

CPP 13.14 Tue 18:15 Poster A

Phase diagram of a diblock copolymer film in an electric field in the strong segregation limit — •Michael Harrach[1], Marianne Heckmann[1], Tiago Peixoto[2], and Barbara Drossel[1] — [1]Institut für Festkörperphysik, TU Darmstadt — [2]Institut für Theoretische Physik, Universität Bremen

We obtain phase diagrams for a thin film of diblock copolymers in an electric field at low temperatures in the strong-segregation limit. In this limit, the system consists of pure A and B domains, and the contributions to the free energy are due to interfacial and polymer stretching effects. We assign different dielectric constants to the two types of domains and evaluate the free energy for different types of phases that are composed of lamellar and cylindrical components, which may be deformed. We consider a two-dimensional system, assuming translational invariance in the third dimension, and periodic boundary conditions in the direction parallel to the condensator plates, between which the polymer film is confined. Specific three dimensional morphologies are considered as well. Phase diagrams are shown as function of film thickness and electric field. Results are presented for a ratio of permittivites of 1:5, for three volume fractions of monomers and four differing field strengths.

CPP 13.15 Tue 18:15 Poster A

Evidence of elastic behaviour of a distorted monolayer — •Uli Langer and Thomas M. Fischer — Uni Bayreuth, Bayreuth, Germany

In our experiment we spread carboxilic particles with a diameter of 100 nm at the air/water interface where they form a monolayer with two phases. Adding nickel nanowires we can excess a shear force by using an external static magnetic field. The nanowires reorient when the external field is switched between x- and y-direction. Located in the denser phase they deform the nearby domains of the less dense phase. While most of the domains start relaxing immediately after the torque was applied some keep their distorted shape until the nanowires are flipped back to their original position.

We computed several physical properties of the monolayer including the line tension λ between the phases, the viscosity η of the denser phase, the pressure difference $\Delta\pi$ between the two phases, and the force density profile acting on a distorted domain.

CPP 13.16 Tue 18:15 Poster A

Interfacial effects on single dye dynamics in ultrathin liquid films and in nanopores — •Fabian Meier, Daniela Täuber, and Christian von Borczyskowski — nanoMA, TU-Chemnitz, Institut für Physik

Nanopores have gained importance as filters in industrial and environmental applications. Thereby interactions of guest molecules are of interest, and thus have led to ongoing research. Here we use single molecule methods to explore the dynamics of dye molecules within nanopores and ultrathin liquid films [1,2] on differently treated silica surfaces. In contrast to ensemble methods, we thereby gain information on a local sub-micron scale. This allows us to draw conclusions on diffusion coefficients and physio-chemical binding affinities depending on the chemical structure of participating molecules and solid surfaces.

[1] D. Täuber, C. von Borczyskowski et al: Diff. Fund. J. 11 (2009) 76.
[2] D. Täuber, Dissertation, TU Chemnitz, 2011.

CPP 13.17 Tue 18:15 Poster A

Increased sorption of water investigating ultrathin polyvinylacetate films — •Heiko Huth and Christoph Schick — Universität Rostock, Institut für Physik, Wismarsche Straße 43-45, 18051 Rostock

Calorimetry is known as a very powerful tool for the characterization of a wide variety of materials and their transitions. There is an ongoing interest in improving the technique in order to achieve high sensitivity and precision. As one example there is thin film ac calorimetry able to measure in the nanometer range [1]. There is also an increasing interest in thin films and small sample sizes from a technological point of view. As these applications often include the presence of water the controlled humidity is used as a new parameter in addition to temperature for calorimetry. Also for biolgical samples as proteins for example there is an interest to measured under controlled humidity [2].

We show a new setup to measure heat capacity of thin films and samples under controlled humidity. As a first example thin films of polyvinylacetate are measured where a large influence of humidity on the glass transition is known from literature. In comparison to bulk samples the glass transition temperature is not changed while an increased sorption of water is observed measuring ultrathin films.

[1] Huth, H., Minakov, A. A., Schick, C., J. Polym. Sci. B Polym. Phys. 44 2996 (2006).

[2] Svanidze, A. V., H. Huth, et al. Applied Physics Letters 95 (26): 263702 (2009).

CPP 13.18 Tue 18:15 Poster A

Functionalization of silicon oxide nanopatterns by selective binding of fluorescent molecules — •Thomas Baumgärtel[1], Christian von Borczyskowski[1], and Harald Graaf[2] — [1]Center of Nanostructured Materials and Analytics, Institut für Physik, TU Chemnitz, 09107 Chemnitz, Germany — [2]FB 10, Institut für Chemie, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

Local anodic oxidation (LAO) of alkyl-terminated silicon is a neat way for generating nanostructures with lateral dimensions below 100 nm and a height of a few nm. One of the remaining challenges is to give those structures a desired functionality in order to build more complex systems. Functionalization can be achieved via different methods such as electrostatic or covalent binding of optically active materials (e.g. molecules or nanoparticles). Here we report on the selective binding of dye molecules to LAO nanostructures and their investigation by means of temporally and spectrally resolved fluorescence microscopy. The spectra of bound perylene dyes have only little similarity to the monomer spectrum, are strongly red-shifted and the radiative transition is characterized by a higher lifetime of the excited state. This can be understood in terms of an oligomer formation of the dyes bound to the nanostructure similar to thin films or stacks of perylene derivatives. Fluorescein dyes that are bound covalently to the oxide on the other hand exhibit a spectrum which is quite similar to the monomer spectrum except of a slight red-shift caused by the different environment. Both systems may be promising candidates for chemically well-defined optically functional nanodevices on semiconductor surfaces.

CPP 13.19 Tue 18:15 Poster A

Mineralisation of iron oxides under lipid monolayers studied by x-ray scattering experiments — •Steffen Bieder[1], Florian Wieland[1], Patrick Degen[2], Michael Paulus[1], Martin Schroer[1], Johannes Möller[1], Christoph Sahle[1], Ralph Wagner[3], Heinz Rehage[2], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, TU Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44227 Dortmund — [2]Physikalische Chemie II, TU Dortmund, Otto-Hahn-Str. 6, D-44227 Dortmund — [3]Fakultät Physik, Bergische Universität Wuppertal, Gaußstr. 20, D-42097 Wuppertal

Composite materials formed by nature show a hierarchically organized and complex structure. The biomineralization processes in living organisms are controlled by proteins and the environment where the process takes place, e.g., the cell interia or the surface of membranes. We studied the mineralization of iron oxide in-situ at the aqueous solution/air interface. As a model system for membranes in living cells we used Langmuir layers consisting of lipids with differently charged headgroups in order to investigate the influence of electrostatic interactions on the mineralization process. The adsorption of iron oxide at the monolayers was observed by grazing incidence diffraction (GID) and extended x-ray absorption fine structure (EXAFS) spectroscopy. We also studied the mineralization with x-ray reflectivity (XRR) experiments at the liquid-liquid interface. The extracted data show an agglomeration of iron oxides at the monolayers. The formation of the growing iron oxides were similar to the formation of lepidocrocite and goethite.

CPP 13.20 Tue 18:15 Poster A

Surface Properties of Catanionic Mixtures — •Heiko Fauser, Martin Uhlig, and Regine v. Klitzing — Stranski-Laboratorium, Department of Chemistry, TU Berlin, Straße des 17. Juni 124 D-10623 Berlin, Germany

Mixtures of oppositely charged surfactants show a strong synergism. It allows reducing the required amount of surfactant, which makes catanionic surfactant mixtures eco-friendly. Thus, these mixtures are of great interest for a broad field of applications like detergency, oil recovery, food technology and drug delivery. Furthermore, foam stability can be increased with these mixtures, since the formation of surface active complexes and aggregates strongly increases the adsorption at liquid-air interfaces.

Literature shows that mixtures of surfactants with unequal chain length have different surface properties in comparison to mixtures with equal chain length. Thus, the focus of our study is on the influence of the surfactant alkyl chain length on the foam properties. In our work catanionic mixtures from two widely used surfactant types, sodium alkyl sulfates and quarternary alkylammonium bromides are investigated. To describe the adsorption of the aggregates at the liquid-air interface both the surface tension and the surface elasticity of mixtures with both matching chain length and mismatching chain length are investigated. Studies about the correlation between adsorbed amount of surfactants, interactions in thin foam films, foam ability and foam stability are in progress.

CPP 13.21 Tue 18:15 Poster A

The role of the solid/liquid interface on the dewetting process of thin polystyrene films — •Mischa Klos[1], Matthias Lessel[1], Oliver Bäumchen[1,2], and Karin Jacobs[1] — [1]Saarland University, Experimental Physics, D-66041 Saarbrücken — [2]Dept. of Physics & Astronomy, McMaster University, 1280 Main St. W, Hamilton, Canada, L8S 4M1

The continuing miniaturization of microfluidic devices causes a growing importance of the solid/liquid interface for the flow dynamics. Our experiments probe slippage using the dewetting process of thin polymer films on hydrophobic substrates. As hydrophobic coatings we use amorphous polymers (AF1600, AF2400) and different types of highly ordered self-assembled silane monolayers on top of ultraflat silicon substrates. Polystyrene (PS) of low molecular weight shows slip lengths between several hundreds of nanometers and even micrometers on silane surfaces [1], whereas on AF1600 nearly no slip is observable. However, slip can be induced by increasing the molecular weight of the PS [2]. Recent studies using scattering techniques showed an ordering effect of PS at the solid/liquid interface depending on the structure of the substrate [3]. Will the situation change if, instead of PS, polymethyl methacrylate (PMMA) is used? To probe the influence of the polymers composition on slippage, we show very first results of the dewetting dynamics of PMMA on AF2400.

[1] R. Fetzer, et. al., Europhys. Let., 75, no. 4, 638 (2006) [2] O. Bäumchen, et al., PRL, 103, 247801 (2009) [3] P. Gutfreund, et. al., arxiv.org 1104.0868v1 (2011, April 5)

CPP 13.22 Tue 18:15 Poster A

Adsorption of supercritical fluids on solids — Sebastian Holz, •Julia Nase, Michael Paulus, Christian Sternemann, Thorsten Brenner, and Metin Tolan — Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund

Adsorption at interfaces is critical for many processes in nature, as formation of gas hydrates, catalysis, or industrial applications like water purification. The formation of an adsorption layer enhances the gas offer significantly and is thus of importance for transport and exchange processes at membranes and interfaces in nature. More than 100 models have been established to describe the various types of adsorption isotherms. Supercritical adsorption, however, is far less understood, though this phenomenon has been known for some time now. It has tremendous importance in industrial applications like high pressure gas storage systems, Supercritical Fluid Chromatography (SFC), and polymer processing. So far, supercritical adsorption was investigated indirectly by volumetric and gravimetric methods in highly porous systems. However, the solid-gas interface with a possible restructuration of the molecules has never been directly measured. The exact density profile along the surface normal can be determined by x-ray reflectometry, a reliable and well adapted technique to determine interfacial structures. We report on results concerning the adsorption of supercritical carbon dioxide on a silicium wafer. Adsorption isotherms below the critical point are compared to the near critical ($T < T_C + 10\text{K}$) and the over critical regime ($T > T_C + 10\text{K}$).

CPP 13.23 Tue 18:15 Poster A

Freezing single molecule dynamics on interfaces and in polymers — •Felix Schmieder, Stefan Krause, and Christian von Borczyskowski — Fakultät für Naturwissenschaften, Technische Universität Chemnitz, D-09107 Chemnitz

During the past decade, probing nano-scale fluctuations within materials by single molecule spectroscopy (SMS) has become a common method. As the observed emission spectra, fluorescence lifetime and polarization are always a result of intramolecular processes and environmental interactions, it is necessary to exactly know about the photophysics of the probe molecules. We report on the freezing of molecular dynamics of quasi-free molecules on surfaces upon lowering of temperature and embedding into a poly(methyl methacrylate) (PMMA) polymer. This has been investigated by measuring heterogeneous line broadening and spectral diffusion of fluorescence emission spectra by means of time dependent SMS using a home-built confocal laser scanning microscope. Thereby changes of optical transition energies could be observed as a result of both intramolecular changes of conformation and dynamics induced externally by the polymer matrix.

CPP 13.24 Tue 18:15 Poster A

Swelling of Polyelectrolyte Multilayers in Ionic Liquid — Nagma Parveen[1,2] and •Monika Schönhoff[1] — [1]Institute of Physical Chemistry, University of Muenster, Corrensstr. 28/30, D-48149 Muenster, Germany — [2]NRW Graduate School of Chemistry, University of Muenster, Wilhelm-Klemm-Str. 10, D-48149 Muenster, Germany

Their controlled thickness and high mechanical stability make Polyelectrolyte Multilayers (PEM) promising ion conducting membranes. Suitable electrolyte solvents could possibly enhance the ionic conductivity for application in Li batteries. Here, the swelling of PEM with Ionic Liquid (IL) is investigated by Quartz Crystal Microbalance (QCM-D). PEM films are prepared with different combinations of polyelectrolyte, employing PSS/PAH, and PSS/PDADMAC. 1-Hexyl-3-methyimidazolium chloride is used here as a room temperature ionic liquid (RTIL). An enhancement of mass coverage and dissipation is found for films in contact with solutions of IL, suggesting incorporation of IL into the films, accompanied by film swelling. The swelling increases linearly with IL concentration. It is reversible at low IL concentrations, while at higher concentrations irreversible film decomposition occurs. The incorporation can be attributed rather to hydrophobic than to ionic interactions, since PDADMAC-containing films swell more strongly. Generally, the overall swelling can be decomposed into a fast and a slow process of IL uptake and chain reorganisation, respectively. Reversibility and stablility limits of PEM in IL solutions are established by these data.

CPP 13.25 Tue 18:15 Poster A

Frequency Response of Polymer Films Made from a Precursor Colloidal Monolayer on a Nanomechanical Cantilever — Ting Liu[1], Sascha Pihan[1], Marcel Roth[1], Markus Retsch[1], Ulrich Jonas[3], Jochen Stefan Gutmann[2], Kaloian Koynov[1], •Hans-Jürgen Butt[1], and Rüdiger Berger[1] — [1]Max-Planck-Institut für Polymerforschung, Mainz, Germany — [2]Institut für Physikalische Chemie, Universität Duisburg-Essen, Essen, Germany — [3]BOMC Laboratory, FORTH IESL, Heraklion, Greece

Nanomechanical cantilevers (NMC) were used for the characterization of the film formation process and the mechanical properties of colloidal monolayers made from polystyrene (PS). Closely packed hexagonal monolayers of colloids with diameters ranging from 400 nm to 800 nm were prepared at the air water interface and then transferred in a controlled way on the surface on NMC. The film formation process upon annealing of the monolayer was investigated by measuring the resonance frequency of the NMC (≈12 kHz). Upon heating of non-crosslinked PS colloids we could identify two transition temperatures. The first transition resulted from the merging of polymer colloids into a film. This transition temperature at 147 ± 3°C remained constant for subsequent heating cycles. We attributed this transition temperature to the glass transition temperature Tg of PS which was confirmed by dynamic mechanical thermal analysis (DMTA) and using the time temperature superposition principle. The second transition temperature (175 ± 3°C) was associated to the end of the film formation process and was measured only for the first heating cycle.

CPP 13.26 Tue 18:15 Poster A

Fabrication of carbon nanomembranes by helium ion beam lithography — •Xianghui Zhang, Henning Vieker, André Beyer, and Armin Gölzhäuser — Fäkultät für Physik, Universität Bielefeld, Postfach 10 01 31, 33501, Germany

A scanning helium-ion microscope (HIM) can be employed as an imaging and metrology tool for nanotechnology. In addition, the helium ion beam is capable of creating nano-sized patterns and it can perform ion milling as commonly done in a focused ion beam (FIB) system. It is known that aromatic self-assembled monolayers (SAMs) can be cross-linked due to electron irradiation and form mechanically stable carbon nanomembranes (CNMs). Here we use a helium ion beam as direct writing tool to cross-link 4'-nitro-1,1'-biphenyl-4-thiol (NBPT) SAMs with arbitrary patterns. The cross-linked SAMs were transferred to either silicon substrates with an oxide layer for optical characterization or transmission electron microscopy (TEM) grids for preparing free-standing CNMs. The required dose for the complete cross-linking with helium ions is quite similar to that with electrons. To determine the feature resolution limit, we prepared dot arrays of CNMs at various doses and 5 nm feature sizes have been achieved. The proximity effect and the sample damage on the nano-scale patterns were also investigated. Furthermore, we use the ion beam to form nanopores in the CNM with an attainable feature size of 5 nm.

CPP 13.27 Tue 18:15 Poster A

Switching properties and orientation of dichroic fluorescent dyes in a nematic liquid crystal — •Clemens Göhler, Harald Graaf, and Christian von Borczyskowski — TU Chemnitz, Institut für Physik

In a liquid crystal cell (LC-cell), the direction of the nematic phase director can be varied by applying an electric field [1]. It is also known that dichroic dye molecules may align with their long molecular axis parallel to the director. While illuminating the LC-cell, fluorescence emission intensity will change due to the applied field and the angle between the dye long molecular axis and its transition dipole moment [2]. By using both principles, a LC-cell with field induced colour switching should be realizable.

We investigate dye molecules that show shape anisotropy caused by long alkyl chains. Thus we manage both a collinear and perpendicular alignment to the transition dipole moment. Using (polarized) fluorescence emission spectroscopy the orientation and order parameter of the dyes within the nematic liquid crystal is determined.

[1] Williams, R.: J. Chem. Phys. 39, 384 (1963)
[2] Heilmeier, G.H, Zanoni, L.A.: Appl. Phys. Letters 13, 91 (1968)

CPP 13.28 Tue 18:15 Poster A

Morphology and rupture forces of liquid gallium immobilized on different surfaces — •Frank Lawrenz[1], Nikolai Severin[2], Jürgen P. Rabe[2], Christiane A. Helm[1], and Stephan Block[3] — [1]Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Str. 6, D-17487 Greifswald, Germany — [2]Department of Physics, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — [3]ZIK HIKE - Zentrum für Innovationskompetenz Humorale Immunreaktionen bei kardiovaskulären Erkrankungen, Fleischmannstr. 42 - 44, D-17487 Greifswald, Germany

Liquid gallium is immobilized on mica, silicon and silica surfaces at 50 °C. AFM tapping mode imaging shows that gallium drops (micrometer-sized) as well as extended layers with nm-thickness and very low roughnesses are formed. Relatively large forces (on the order of several 10 nN) have to be applied to immerse a silicon tip (curvature radius around 10 nm) into the micrometer-sized gallium droplets. The forces exhibit many rupture events. The distribution of the rupture length is very broad and has a maximum at around 0.25 nm. It is most likely, that (solid) sheets of amorphous gallium oxide is formed at the air/liquid interface of gallium drops. These sheets interact with the AFM tip leading to the observed rupture events. Moreover, they are transferred during the preparation procedure to the surface forming the flat layers with nm-thickness.

CPP 13.29 Tue 18:15 Poster A

Interactions of Radical Oxygen Species with Phosphatidylcholine Monolayers and Liposomes — •Andreas Gröning[1], Heiko Ahrens[1], Frank Lawrenz[1], Thomas Ortmann[1], Gerald Brezesinski[2], Fritz Scholz[3], Doris Vollmer[4], and Christiane A. Helm[1] — [1]Institut für Physik, Uni Greifswald, 17487 Greifswald, Germany — [2]MPI KGF, 14476 Potsdam, Germany — [3]Institut für Biochemie, Uni Greifswald, 17487 Greifswald, Germany — [4]MPI P, Ackermannweg 10, 55128 Mainz, Germany

The reaction of phosphatidylcholines with hydroxyl radicals is investigated. The radicals are produced by the Fenton reaction. The radical concentration is varied. For DPPC monolayers a decrease in the lateral pressure is used as a measure of the efficiency of the radical attack. Combining isotherms and X-ray diffraction we find that the monolayer can be compressed to smaller molecular areas, with a reduced tilt angle of the alkyl chains. Consistent with this observation IRRAS experiments indicate a partial cleavage of the head group leading to a reduced head group size. X-ray reflectivity demonstrates Fe^{2+} binding to the head group. Fluorescence microscopy during the radical attack shows that new domains in the condensed phase nucleate immediately.

Furthermore, DMPC liposomes are investigated with differential scanning calorimetry. With increasing radical concentration, the alkyl chain melting transition is shifted to higher temperatures. Summarising, we observe solidification for both monolayers and liposomes which we attribute to a preferential radical attack on the hydrophilic head group region, followed by Fe^{2+} binding.

CPP 13.30 Tue 18:15 Poster A

Can we correlate residual stresses in ultrathin polymer films with a high surface mobility? — •Mithun Chowdhury[1], Paul Freyberg[1], and Günter Reiter[1,2] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, 79104, Freiburg, Germany — [2]Freiburg Institute for Advanced Studies (FRIAS), 79104, Freiburg, Germany.

The fabrication process of a thin polymer film, involving the transition from a solution to a glass, is believed to have an impact on film properties, often related to poorly entangled out-of-equilibrium chain conformations and corresponding residual stresses caused by rapid solvent loss. Physical ageing of polymer films, at temperatures below the glass transition was found to lead to a progressive decay in dewetted hole size (indicative of a decreasing residual stress), in a close to exponential fashion with ageing time, defining a characteristic relaxation time. Relaxation times are largely in agreement with some earlier reports based on surface sensitive techniques for thin polymer films. This is indeed surprising as dewetting cannot be considered as a surface sensitive probe. Moreover, temperature dependence of the relaxation time of residual stresses, above the glass transition of the polymer can be obtained from the evolution of the shape of the dewetting rim. Relaxation times in that region are much faster with a significant deviation from the bulk polymer. Our results certainly invoke the possibility to explain the faster relaxation dynamics in thin films and its deviation from the bulk, also in terms of residual stresses induced from the film preparation stage.

CPP 13.31 Tue 18:15 Poster A

Modification of wrinkled surfaces through defects — •Patrick Wünnemann[1], Marco Phillip Schürings[1], Felix Plamper[2], Andrij Pich[3], and Alexander Böker[1] — [1]DWI an der RWTH Aachen, Lehrstuhl für Makromolekulare Materialien und Oberflächen, RWTH Aachen, D-52056 Aachen, Germany — [2]IPC an der RWTH Aachen, Lehrstuhl für Physikalische Chemie, RWTH Aachen, D-52056 Aachen, Germany — [3]DWI an der RWTH Aachen, Funktionale und Interaktive Polymere, RWTH Aachen, D-52056 Aachen, Germany

We verify the effects of defects introduced to soft Poly(dimethylsiloxane) (PDMS) substrates through the formation of wrinkle structures to develop new patterns of wrinkled surfaces. These stress induced disruptions lead to star-like wrinkled sufaces on the nanoscale. Next to the effects of single defects we investigate wrinkled structures in the area between adjacent defects. First description of the domains, the wavelength and the induced pattern in the vicinity of the nanodefects are characterized by scanning force microscopy (SFM). The focus of our work is the correlation between wavelength and thickness of the oxidized PDMS-surface and the applied strain. Compared to other systems these defects are more likely to be fabricated by lithographic methods. We further study the possible use as a template for the two-dimensional arrangement of soft matter particles.

CPP 13.32 Tue 18:15 Poster A

Phase transitions of Polypeptides in confined geometries — •Renate Reiter[1], Frédéric Wintzenrith[2], and Günter Reiter[1] — [1]Physikalisches Institut, Universität Freiburg, Germany — [2]Ecole Polytechnique, France

Poly-γ-benzly-glutamte (PBLG) is a synthetic polypeptide which can adopt α-helical conformation in aprotic solvents and thus forms rigid rods with flexible side chains. The experimentally observed phase diagram in organic solvents corresponds well to the theoretical one of Flory which predicts a coexistence region of isotropic, liquid crystalline and network phases. Networks were observed experimentally by cooling the isotropic phase to the transition temperature followed by quenching.

We demonstrate that quasi two dimensional network like structures are obtained by preparing Langmuir films of PBLG from helicogenic solvent. With this technique molecules are confined to the air water interface and changing the molecular density via movable barriers allows inducing phase transitions which appear as discontinuities in the isotherms. BAM and AFM micrographs reveal fibrils and networks directly on the water surface and in films transferred to solid substrates. Unusual hysteric and relaxation behavior of the isotherms are observed and discussed. A correlation between morphological changes and phase transitions is targeted.

CPP 13.33 Tue 18:15 Poster A

Controlling Colloidal Self-Assembly with Gradient Wrinkle Substrates in Combinatorial Experiments — Stephanie Hiltl, Jens Oltmans, and •Alexander Böker — DWI an der RWTH Aachen e.V., Lehrstuhl für Makromolekulare Materialien und Oberflächen, RWTH Aachen, D-52056 Aachen, Germany

We prepare wrinkle gradients in oxidized top layers on elastic poly(dimethylsiloxane) (PDMS) substrates covering several millimeters of the sample. While the amplitude of the gradient structure ranges from 7-230 nm, the wavelength spans several hundred nanometers (250-900 nm). Crucial for the gradient preparation is partial shielding of the PDMS sample during plasma oxidation. We take advantage of the newly developed surface geometry for combinatorial experiments regarding the assembly of microgels as a model particle system. By variation of the ratio of particle radius vs. wrinkle wavelength, we scan and optimize the influence of the wrinkle dimensions on particle shape, particle-sample interaction and the particle assembly in a single experiment.

CPP 13.34 Tue 18:15 Poster A

Modelling surfactant covered films - thermodynamic reformulation and extension of the hydrodynamic evolution equations — •Uwe Thiele[1], Andrew J. Archer[1], and Plapp Mathis[2] — [1]Department of Mathematical Sciences, Loughborough University, Loughborough, Leicestershire, LE11 3TU, UK — [2]Physique de la Matiere Condensee, Ecole Polytechnique, CNRS, 91128 Palaiseau, France

We propose several models that describe the dynamics of liquid films that are covered by a relatively large concentration of insoluble surfactant. First, we briefly review the 'classical' hydrodynamic form of the coupled evolution equations for film height and surfactant concentration that are well established for small concentrations. Then we re-formulate the basic model as a gradient dynamics based on an underlying free energy functional that accounts for wettability and capillarity. Based on this re-formulation in the framework of non-equilibrium thermodynamics, we propose extensions of the basic hydrodynamic model that account for (i) nonlinear equations of state, (ii) surfactant-dependent wettability, (iii) surfactant phase transitions, and (iv) substrate-mediated condensation. In passing we discuss important differences to models found in the literature.

We acknowledge support by the EU (PITN-GA-2008-214919).

CPP 13.35 Tue 18:15 Poster A

Layer thickness homogeneity determination via Rutherford backscattering in helium-ion microscopy — •Henning Vieker, Karsten Rott, André Beyer, Günter Reiss, and Armin Gölzhäuser — University Bielefeld, Faculty of Physics, Germany

The recently developed helium-ion microscope allows remarkable surface resolution with the secondary-electron (SE) detector. Simultaneously, backscattered ions can be detected that allow imaging with a substantially higher elemental contrast. This Rutherford backscattered (RBS) ion contrast depends mainly on the elemental composition of the investigated sample surface. The escape depth of RBS ions is much larger than for secondary electrons. Thus whole layers with a wide range of thicknesses will contribute to a RBS ion image, whereas the SE image is far more surface sensitive, i.e. insensitive to buried parts under the sample surface.

In this contribution we examine RBS ion imaging as tool to characterize thickness variations of layered samples with well defined compositions. In a model example the homogeneity of gold layers on silicon substrates is investigated. Achievable spatial resolutions as well as the possibilities in using a reference sample to measure layer thicknesses will be addressed.

CPP 13.36 Tue 18:15 Poster A

Site specific electronic structure of electron doped $SrTiO_3$ and $SrTiO_3$ /$LaAlO_3$ interfaces — •Christoph Schlueter[1], Tien-Lin Lee[2], Carmela Aruta[3], and Jörg Zegenehagen[1] — [1]ESRF,Grenoble, France — [2]Diamond Light Source Ltd, Didcot, UK — [3]CNR-SPIN, Naples, Italy

A quasi-2dimensional electron gas is formed at the interface of the insulation oxides SrTiO3 (STO) and LaAlO3 (LAO). Despite significant research efforts the origin of the conductivity is still heavily discussed. This electron gas is expected to occupy states up to the Fermi level.

We present results of hard X-ray photoelectron spectroscopy (HAXPES) measurements on the STO/LAO hetero structures in comparison to electron doped single crystalline STO samples. Additional information is added by combining HAXPES with the site specific X-ray standing wave effect. This gives the possibility to decompose the spectra into the relative contributions from different lattice sites. Hence, coherent and incoherent (delocalized/localized) states close to the Fermi level can be distinguished. The obtained spectra show a partial filling of Ti d-bands, crossing the Fermi level. Oxygen deficient samples exhibit an additional incoherent peak +1.3eV below the Fermi level. For the hetero structures we identified carriers at the Fermi level from the conductive interface region and give experimental evidence of partial filling of Ti 3d bands and the presence of the oxygen vacancy related incoherent peak.

CPP 14: Poster: Glasses I (jointly with DY)

Time: Tuesday 18:15–20:15 Location: Poster A

CPP 14.1 Tue 18:15 Poster A

Elastic Properties of Amorphous Solids — •Christian L. Klix, Florian Ebert, Georg Maret, and Peter Keim — University of Konstanz

In this contribution, we present experimental results on the elastic properties of a two-dimensional colloidal glass former. Given that glasses are solids, one expects a mechanical behavior similar to that of crystals, i.e., glasses exhibit a finite shear modulus μ. Using positional data from video microscopy, we study the displacement field and connect it to the dynamical matrix $D(q)$ via the equipartition theorem [1]. The resulting dispersion relation of the system hints at structural change upon decreasing the temperature in the glassy state. Next, this data is used to derive the Lamé coefficients and the corresponding moduli from thermally excited modes in the long wavelength limit [1] using continuum elasticity theory. We consider finite size and time effects and find the expected frequency dependence of the shear modulus μ. By cooling the system, the significant increase of μ allows us to determine the glass transition temperature T_g precisely. Following the method described in [2], we compute the short wavelength excitations in our system and analyse the density of states as well as the structure of normal modes in a two-dimensional colloidal system.

[1] H. H. Von Grünberg, P. Keim, and G. Maret, Phys. Rev. Lett. 93, 255703 (2004)

[2] A. Gosh, V. K. Chikkadi, P. Schall, J. Kurchan, and D. Bonn, Phys. Rev. Lett. 104, 248305 (2010)

CPP 14.2 Tue 18:15 Poster A

Segmental and chain dynamics of polyisoprene confined in thin layers — •Emmanuel Urandu Mapesa, Martin Tress, and Friedrich Kremer — Institute for Experimental Physics I, University of Leipzig, 04103 Leipzig, Germany

Broadband Dielectric Spectroscopy (BDS) - in combination with a nanostructured electrode arrangement - is used to study thin layers of cis-1,4-polyisoprene (cis-PI). cis-PI belongs to a special type of polymers because a part of its molecular dipole moment attached to each monomer unit is aligned along the main chain. This fraction adds up to one dipole moment of the whole polymer chain corresponding to the end-to-end vector of the molecule. Consequently, the investigation of two distinct relaxation modes taking place at two different length scales is possible: the segmental motion which involves structures of about one nanometer in size, and the normal mode which represents the dynamics of the whole macromolecule. In the current study, where highly insulating silica nanostructures are used as spacers, the need to evaporate a counter-electrode is circumvented. The spin-cast samples are checked before and after dielectric measurement so as to exclude the possibility of dewetting affecting the measured dynamics. Down to 7 nm, for three molecular weights (44.5, 53 and 75 kg/mol), it is observed that: (i) the segmental mode (and hence the dynamic glass transition) is unaffected by 1-D confinement, and (ii) the normal mode becomes faster with decreasing layer thickness in dependence on molecular weight.

CPP 14.3 Tue 18:15 Poster A

Holographic Studies of New Azobenzene-Containing Low-Molecular-Weight Phase-Change Materials — •Christoph Meichner[1], Lothar Kador[1], Christian Probst[2], and Hans-Werner Schmidt[2] — [1]University of Bayreuth, Institute of Physics and Bayreuther Institut für Makromolekülforschung (BIMF), 95440 Bayreuth, Germany — [2]University of Bayreuth, Macromolecular Chemistry I and Bayreuther Institut für Makromolekülforschung (BIMF), 95440 Bayreuth, Germany

Using a plane-wave holographic setup, we investigated new azobenzene-containing low-molecular-weight materials which reveal a light-induced phase change from glassy to liquid-crystalline. Different parameters such as refractive-index modulation, long-term stability, writing speed, and sensitivity have been measured for different mixing ratios between the photo-active material and a similar but inactive compound. The experiments demonstrated that the inactive compound showed partial reorientation effects, which were driven by the *trans-cis-trans* isomerization cycles of the azobenzene moieties. In addition, an improved setup for the parallel inscription and reconstruction of two-dimensional data pages was built to test the feasibility of fast and high-density data storage. It is based on an LCD spatial light modulator and high-quality camera objectives.

CPP 14.4 Tue 18:15 Poster A

Heat capacity spectroscopy of the dynamic glass transition in chosen room temperature ionic liquids — •Evgeni Shoifet[1], Heiko Huth[1], Sergey Verevkin[2], and Christoph Schick[1] — [1]University of Rostock, Institute of Physics, 18051 Rostock, Germany — [2]University of Rostock, Institute of Chemistry, 18051 Rostock, Germany

Many of the ionic liquids are good glass formers. Nevertheless, only a few studies of the glass transition in ionic liquids are available so far. Particularly the frequency dependence of the dynamic glass transition (alpha-relaxation) is not known for most ionic liquids. The standard technique for such studies - dielectric spectroscopy - is not easily applicable to ionic liquids because of the high electrical conductivity. The aim of this study is to use different calorimetric techniques to obtain complex heat capacity and to investigate the dynamic glass transition of room temperature ionic liquids (RTILs) in a wide frequency range. This can give an insight in cooperative motions of ions and ion clusters in RTILs. The techniques that were used are DSC, TMDSC, and AC-chip calorimeter covering a total range of 0.001-10000 Hz. The trace of the dynamic glass transition in the activation diagram for RTILs was fitted to the Vogel-Fulcher-Tammann-Hesse function and the parameters compared for different RTILs.

CPP 14.5 Tue 18:15 Poster A

Differential AC chip calorimeter for in situ investigation of

vapor-deposited thin films — •Mathias Ahrenberg[1], Evgeni Shoifet[1], Katie Whitaker[2], Heiko Huth[1], Mark Ediger[2], and Christoph Schick[1] — [1]Universität Rostock, Institut für Physik, Universitätsplatz 3, 18055 Rostock — [2]Department of Chemistry, University of Wisconsin - Madison, Madison, Wisconsin 53706, USA

Physical vapor deposition (PVD) can be used to produce thin films with interesting material properties including extraordinarily stable organic glasses. We describe an AC chip calorimeter for in-situ heat capacity measurements of as-deposited nanometer thin films of organic glass formers. The calorimetric system is based on a differential AC chip calorimeter which is placed in the vacuum chamber for physical vapor deposition. The sample is directly deposited onto one calorimetric chip sensor while the other sensor is protected against deposition. The device and the temperature calibration procedure are described. The latter makes use of the phase transitions of cyclopentane and the frequency dependence of the dynamic glass transition of toluene and ethylbenzene. Sample thickness determination is based on a finite element modeling (FEM) of the sensor sample arrangement. In the modeling, a layer of toluene was added to the sample sensor and its thickness was varied in an iterative way until the model fit the experimental data.

CPP 14.6 Tue 18:15 Poster A

High-frequency laser modulated AC-chip calorimetry investigations of glass transition of polymers — •Yeong Zen Chua, Evgeni Shoifet, Gunnar Schulz, and Christoph Schick — Universität Rostock, Institut für Physik, Wismarsche Straße 43-45, 18051 Rostock, Germany

Combination of different techniques for heat capacity spectroscopy and temperature-modulated calorimetry allows the determination of complex heat capacity in a wide frequency range. We study the dynamic glass transition and its corresponding temperature-dependent cooperativity of polymers. An AC-chip calorimeter gives the possibility to decrease the size of the measured sample, hence increases the sensitivity and frequency range. However, the investigation of the dynamic glass transition is still limited to the frequencies up to a few kHz, due to capacitive coupling between heater driving voltage and thermopile voltage at high frequencies. A new AC-chip calorimeter with laser heating, which decouple the temperature measurement and heating, is capable of measuring the glass transition temperature of thin film samples in nanogram range and in the frequency range up to 500 kHz. The dynamic glass transition of polystyrene and poly(methyl methacrylate) was studied from 10^{-5} Hz to 500 kHz.

CPP 14.7 Tue 18:15 Poster A

Molecular dynamics of glass forming liquids confined in two dimensional constraint of uni-directional nanopores — •Wycliffe Kipnusu, Ciprian Iacob, Joshua Sangoro, and Friedrich Kremer — Institute of Experimental Physics I, University of Leipzig, Linnestr. 5, 04103 Leipzig, Germany.

Broadband Dielectric Spectroscopy (BDS), Pulse Field Gradient-Nuclear Magnetic Resonance (PFG-NMR) spectroscopy, and Fourier Transform Infrared (FT-IR) spectroscopy are combined to study the molecular dynamics of low molecular weight glass forming liquids (e.g. alkylcitrates) in the bulk state and confined in unidirectional nanopores (diameter: 4, 8, and 10.4 nm, length: 50 microns) prepared by electrochemical etching of highly doped p-type $< 100 >$ silicon and subsequent oxidation. The dynamics of the structural (alpha)relaxation and the diffusion are enhenced by more than 2 orders of magnitude in 4 nm pores at lower temperatures in comparison to the bulk. This is attributed to changes in molecular packing due to geometrical constraint. Apart from a beta- relaxation, a broad process (slower than the alpha- process) assigned to relaxation of interfacial layers is observed for the confined molecules. Silanization of the pores removes this process but does not alter the structural alpha- relaxation.

References:

(1). M. Arndt, etal. Physical review. E, 1996, 54, 5377. (2). F. Kremer Broadband Dielectric Spectroscopy, Springer, Berlin, 2003. (3). R. Prisk, and P. E. Sokol, J. Chem. Phys., 2011, 134, 114506

CPP 14.8 Tue 18:15 Poster A

Shear moduli of two dimensional binary glasses — •Rabea Seyboldt[1], David Hajnal[2], Fabian Weysser[1], and Matthias Fuchs[1] — [1]FB Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany

We studied the shear moduli of two-component glasses in two dimensions within mode coupling theory. Varying the concentration, strong mixing effects can be observed along the glass transition lines for two interaction potentials. Hard disks with size ratios between 0.3 and 0.9, and point particles interacting with (magnetic) dipoles of strength ratio between 0.1 and 0.6 are considered. Equilibrium structure factors (partially obtained from Monte Carlo simulations) and glass form factors show that a softening of the elastic shear constant of glass upon adding another component arises from a dilution effect of the majority component. For very disparate mixtures, an anomalous elastic strengthening results from what we interpret as clustering of the smaller particles in the voids between the larger ones. This among other things might indicate a close-by glass-glass transition. Simulation data on hard disk mixtures show that the theory underestimates the moduli by around 50%, but otherwise captures the qualitative trends (within the rather large simulational error bars).

CPP 14.9 Tue 18:15 Poster A

Excess heat capacity and fictive temperature of polystyrene in a wide range of cooling and heating rates — •Gunnar Schulz[1], Timur V. Tropin[2], Jürn W. Schmelzer[1], and Christoph Schick[1] — [1]University of Rostock, Institut of Physics, 18055 Rostock, Germany — [2]Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, 141980 Dubna, Russia

The physical characteristics of polystyrene allow us straightforward and reproducible measurements of heat capacity, C_p, glass transition temperature, T_g, and other properties. The possibility to reuse one sample for numerous cooling and heating cycles permits the investigation of the influence of the cooling and heating rates on C_p and T_g.

In our research, we conduct the cooling phases with various (constant) cooling rates, but the respectively following heating phases with only one heating rate. The comparison of the heat capacities observed after different cooling rates results in an excess C_p, which we also calculate by means of an appropriate model.

Our measurements furthermore yield the fictive temperature in the cooling rate range from 10^{-4} Ks^{-1} to 10^4 Ks^{-1}. We compare these results with the dynamic T_g observed by means of temperature-modulated differential scanning calorimetry (TMDSC). The dependence of the fictive T_g on the cooling rate and the dependence of T_g on the modulation frequency turn out to be closely related.

CPP 14.10 Tue 18:15 Poster A

Dielectric relaxation of alcohols in silica nanochannels — •Daniel Rau, Carsten Biehl, Rene Berwanger, and Rolf Pelster — Experimentalphysik, Universität des Saarlandes

We studied the molecular dynamics and glass transition of n-butanol and 2-ethyl-1-hexanol confined in silica nanochannels using broadband dielectric spectroscopy. For this purpose we have varied the pore radii in the range from 3 to 7 nm[1]. In contrast to the bulk material, confined n-butanol exhibits a glass transition upon slow cooling. Interestingly, in larger pores partial recristallization occurs upon heating. This behaviour reflects the different temperature dependence of nucleation and crystal growth.

[1] Berwanger et al., Eur. Phys. J. Special Topics 189, 239-249 (2010)

CPP 14.11 Tue 18:15 Poster A

Probing a statical, critical length scale in supercooled liquids — •Ingo Füreder, Patrick Ilg, and Hans Christian Öttinger — ETH Zürich, Switzerland

Nonequilibrium molecular simulations of glassy systems pose several challenges due to their long relaxation times and the large time scale gap between micro- and macroscopic dynamics. Guided by general principles of nonequilibrium thermodynamics we develop a constitutive model which should enable us to describe the behaviour of supercooled liquids in a quantitative manner on a macroscopic scale. The building blocks of the model contain a naturally arising length scale in glassy systems being a signature of growing amorphous order near the glass transition. This length is associated with the hindrance of affine deformations of an inherent structure configuration and could be extracted by investigating the system's non-affine response to static shear.

CPP 14.12 Tue 18:15 Poster A

Molecular signature of the dynamic glass transition as probed by spectroscopies sensing inter- and intra-molecular interactions — •Wilhelm Kossack[1], Periklis Papadopoulos[2], and

Friedrich Kremer[1] — [1]Fakultät für Physik und Geowissenschaften, Linnéstraße 5, 04103 Leipzig, Germany — [2]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany

The dynamic glass transition reflects a continuous slowing down of relaxations between structural substates of a glass forming system. Conventially its temperature dependence is described by the empirical Vogel-Fulcher-Tammann dependence. In the present study Fourier Transform InfraRed (FTIR) spectroscopy is employed to study the inter-molecular interactions between different molecular moieties of glass forming systems by measuring the temperature dependence of the spectral positions of its characteristic vibrations. In combination with Broadband Dielectric Spectroscopy (BDS) and DC- and AC- calorimetry this delivers a novel detailed insight into the molecular signature of the dynamic glass transition being specific for each glass forming system.

CPP 14.13 Tue 18:15 Poster A

Space-time phase transition in an atomistic model of glass formers — •Thomas Speck — Institut für Theoretische Physik II, Heinrich-Heine-Universität Düsseldorf, Germany

The transformation of a liquid into a solid crystal is a first-order phase transition that occurs through nucleation. All liquids can, therefore, be supercooled to a certain degree; and some turn into highly viscous, amorphous solids. One of the striking features is the emergence of dynamic heterogeneity, i.e., while overall particle motion becomes more and more restricted small regions of activity persist. Here we study ensembles of trajectories for a popular atomistic glass former, the Kob-Andersen binary Lennard-Jones mixture. We characterize mobility in a single trajectory through the number of particles that undergo a long-lived displacement. These excited particles record the underlying excitations that lead to dynamic heterogeneity. Using umbrella sampling we determine the probability distribution of this order parameter and show that it is non-concave. This can be interpreted as a phase transition in space-time between an active, liquid-like phase and an inactive, jammed phase in which the system remembers its initial conditions over the observation time. Structural and dynamical properties of these two distinct dynamic phases are analyzed and consequences for the glass transition are discussed.

CPP 14.14 Tue 18:15 Poster A

Differential AC chip calorimeter for in situ investigation of vapor-deposited thin films — •Mathias Ahrenberg[1], Evgeni Shoifet[1], Katie Whitaker[2], Heiko Huth[1], Mark Ediger[2], and Christoph Schick[1] — [1]Universtät Rostock, Institut für Physik, Universitätsplatz 3, 18055 Rostock — [2]Department of Chemistry, University of Wisconsin - Madison, Madison, Wisconsin 53706, USA

Physical vapor deposition (PVD) can be used to produce thin films with interesting material properties including extraordinarily stable organic glasses. We describe an AC chip calorimeter for in-situ heat capacity measurements of as-deposited nanometer thin films of organic glass formers. The calorimetric system is based on a differential AC chip calorimeter which is placed in the vacuum chamber for physical vapor deposition. The sample is directly deposited onto one calorimetric chip sensor while the other sensor is protected against deposition. The device and the temperature calibration procedure are described. The latter makes use of the phase transitions of cyclopentane and the frequency dependence of the dynamic glass transition of toluene and ethylbenzene. Sample thickness determination is based on a finite element modeling (FEM) of the sensor sample arrangement. In the modeling, a layer of toluene was added to the sample sensor and its thickness was varied in an iterative way until the model fit the experimental data.

CPP 14.15 Tue 18:15 Poster A

Phase diagram of confined hard sphere glasses — •Suvendu Mandal[1], Dierk Raabe[1], and Fathollah Varnik[1,2] — [1]Max-Planck Institut fur Eisenforschung, Max-Planck Str. 1, 40237 Dusseldorf, Germany — [2]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universitat Bochum, Stiepeler Strasse 129, 44801 Bochum, Germany

Spatial confinement is known to induce a dramatic change in the viscosity and relaxation time of liquids near the glass transition point (see, e.g., the topical review in [1] and references therein). While this issue has been the subject of a large number of studies for polymers and molecular glasses, only few investigations focus on colloidal hard sphere systems [2]. Quite recently, computer simulation studies of a monodisperse hard sphere (HS) system revealed an oscillatory behavior of the diffusion coefficient as the wall-to-wall distance, H, was varied between 2 and 4 particle diameters [3]. Suppressing crystallization via polydispersity, we extend these studies to considerably higher volume fractions, thereby addressing, for the first time in simulations, the effect of confinement on the mode coupling critical volume fraction. Our results are in good agreement with recent theoretical predictions [4]. A thorough test of other aspects of theoretical predictions is also provided [5].

[1] J. Baschnagel, F. Varnik, J. Phys.: Condens. Matter 17, R851-R953 (2005). [2] C. R. Nugent et al. PRL 99, 025702 (2007). [3] J. Mittal et al. PRL 100, 145901 (2008). [4] S. Lang et al. PRL 105, 125701 (2010). [5] S. Mandal et al. in preparation.

CPP 14.16 Tue 18:15 Poster A

Aging and elementary relaxation processes in amorphous solids — •Nima Hamidi Siboni[1,3], Fathollah Varnik[2], and Dierk Raabe[3] — [1]Aachen Institute for Computational Engineering Science, Aachen, Germany — [2]The Interdisciplinary Centre for Advanced Materials Simulation, Bochum, Germany — [3]Max-Planck Institut für Eisenforschung, Düsseldorf, Germany

Aging affects both dynamical [1] and mechanical (e.g., yield stress [2]) properties of amorphous solids. We study here aging effects on the distribution of elementary relaxation processes for the case of a binary Lennard-Jones glass. Both the distribution of first relaxation events, $\xi(t_1)$, and the waiting time between two successive events, $\phi(\tau)$ is modified upon aging. This is at first sight not surprising since these two distributions are known to satisfy the relation $\xi(t_1) = \int_{t_1}^{\infty} \phi(t')t'dt'/\langle\tau\rangle_\phi$, where $\langle\tau\rangle_\phi = \int_0^{\infty} \phi(t')t'dt'$ is the mean waiting time [3]. Recent simulation studies of this issue, however, report that only $\xi(t_1)$ changes upon aging, while $\phi(\tau)$ seems to remain stationary [4]. This unexpected behavior has been attributed to a possible power-law tail of $\phi(\tau)$ and the resulting divergence of $\langle\tau\rangle$. We thoroughly study this issue and propose possible explanations of this apparent discrepancy [5].

[1] W. Kob, J.-L. Barrat, Phys. Rev. Lett. 78, 4581 (1997).

[2] F. Varnik, L. Bocquet, J.-L. Barrat, J. Chem. Phys. 120, 2788 (2004).

[3] O. Rubner, A. Heuer 78, 011504 (2008).

[4] M. Warren, J. Rottler 88, 58005 (2009).

[5] N. Hamidi Siboni, D. Raabe, F. Varnik (in preparation).

CPP 14.17 Tue 18:15 Poster A

THz dynamics in glasses studied by means of Inelastic Neutron Scattering — •Nicolo' Violini — Jülich Center of Neutron Scattering, Forschungszentrum Jülich, D-52425 Jülich, Germany — Dipartimento di Fisica, Universitá di Perugia, Via A. Pascoli, I-06123, Perugia, Italy

The THz dynamics of two different glasses has been studied by means of Inelastic Neutron Scattering: the germanium diselenide (v-GeSe2) [1], an amorphous glass belonging to the family of continuous random network forming glasses and the glucose (C6H12O6). In both cases two well-defined peaks are resolved in the dynamic structure factor in a broad Q region, below and above the position of the first sharp diffraction peak in the static structure factor. Their common characteristics and possible differences will be discussed during the talk. The presence of two pseudo-branches in glasses seems to be quite general, but their nature is not completely understood, mainly due to the lack of theoretical models able to provide a complete description of this intriguing features[3].

[1] L. Orsingher, G. Baldi, A. Fontana, L. E. Bove, T. Unruh, A. Orecchini, C. Petrillo, N. Violini and F. Sacchetti Phys. Rev. B 82, 115201 (2010).

[2] N. Violini and F. Sacchetti, paper in preparation (unpublished).

[3] N. Violini, PhD Thesis (2011).

CPP 15: Poster: New Instruments and Methods

Time: Tuesday 18:15–20:15 Location: Poster A

CPP 15.1 Tue 18:15 Poster A

Investigating microfluidics at interfaces with GISAXS — •Volker Körstgens[1], Kuhu Sarkar[1], Martin Trebbin[2], Matthias Schwartzkopf[3], Adeline Buffet[3], Stephan V. Roth[3], Stephan Förster[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]Universität Bayreuth, Physikalische Chemie I, 95447 Bayreuth, Germany — [3]HASYLAB at DESY, 22603 Hamburg, Germany

X-rays are a powerful probe for the investigation of flow and processes in microfluidic systems. In pioneering experiments it has been shown that with GISAXS (grazing incidence small angle x-ray scattering), using a specially designed microfluidic cell, surface sensitive investigations are also possible [1]. With the highly brillant x-ray beam available at the beamline MiNaXS of the PETRA III synchrotron source a time resolved as well as a position resolved GISAXS investigation of structural changes at the surface in contact with the flowing liquid becomes possible. The microfluidic cell design offers versatile options including mixing experiments and chemical reactions. Swelling processes, the attachment of particles and also the detachment of unwanted detrimental films can be investigated. The envisaged high time resolution will allow to follow the corresponding kinetics.

This work has been financially supported by the BMBF (grant number 05K10WOA).

[1] J.-F. Moulin et al., Rev. Sci. Instrum. 79, 015109 (2008).

CPP 15.2 Tue 18:15 Poster A

The small angle scattering beamline BW4 of HASYLAB: Recent developments and future perspectives — •Jan Perlich, Jan Rubeck, Stephan V. Roth, and Rainer Gehrke — HASYLAB-DESY, Notkestr. 85, D-22603 Hamburg (Germany)

The small angle scattering beamline BW4 of HASYLAB, Hamburg (Germany), is a dedicated materials science beamline. The main experimental techniques are transmission small angle X-ray scattering (SAXS) as well as grazing incidence small angle X-ray scattering (GISAXS) in reflection geometry. The implemented microfocus option at the BW4 instrument [1] enables experiments where lateral scanning of sample materials is feasible. After major refurbishments of the beamline in the recent years, the focus is on expanding the experimental capabilities by the access to an extended scattering q-range, e.g. GIWAXS [2], and the introduction of necessary sample environments for the structural characterization of novel material systems at specific physical conditions. In addition, in-situ sample observations are possible with a fast detector enabling the structural characterization of time-dependent processes. We present the novel experimental capabilities based on selected recent results [3]. Based on the outstanding performance of this beamline for 20 years, BW4 will remain unforgotten!

[1] Roth et al., Rev. Sci. Instrum. 77 (2006), 085106.

[2] Perlich et al., Rev. Sci. Instrum. 81 (2010), 105105.

[3] Perlich et al., Phys. Status Solidi RRL 3(4) (2009), 118.

CPP 15.3 Tue 18:15 Poster A

A novel Dilatometer to investigate the influence of pressure, cooling rate and shear rate on the specific Volume of polymers. — •Sibylle Jilg, Reinhard Forstner, and Wolfgang Stadlbauer — Transfercenter für Kunststofftechnik GmbH, Franz-Fritsch-Straße 11, 4600 Wels, Austria

These novel pvT-Dilatometer (Pirouette-pvT-Apparatus) was designed to measure the specific volume of polymers under processing conditions as found in injection moulding. So it is possible to investigate the specific volume as a function of temperature (up to 300°C), pressure (up to 1000 bar), cooling rate (up to 100°C/s) and shear rate (up to 180 1/s). The Pirouette is a combination of a traditional piston-die dilatometer and a Couette rheometer. This dilatometer can be used in several operating modes. Isobaric heating, isobaric cooling and isothermal experiments are possible. In this investigation measurements were performed with isotactic Homo-Polypropylenes in the isobaric cooling mode to show the dependency of the transition temperature from pressure, cooling rate and shear flow. It can be found that increasing pressure shifts the transition temperature to higher temperatures and higher cooling rates shifts the transition temperature to lower values. Higher shear temperatures shift the transition temperature to higher temperatures and higher pressures enhance the effect of shear. The specific volume after cooling to room temperature is mainly depending on cooling rate.

CPP 15.4 Tue 18:15 Poster A

Characterization of AFM tips using graphite steps — •Friedrich Lüders, Ann-Kristin Löhmann, and Thomas Thurn-Albrecht — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Germany

To investigate the morphology and mechanical characteristics of soft polymer samples on the nanometer scale, Atomic Force Microscopy (AFM) in Intermittent Contact Mode (ICM) is a commonly used technique. The AFM image is always a convolution of the surface topography and the shape of the tip. The resolution of an image is therefore limited by the sharpness of the tip. Also in ICM the tip indents into the sample, into softer areas more than in harder regions. For a quantitative analysis of AFM images the exact shape of the tip must be known.

We present a simple method for characterization of an AFM tip by scanning the steps between different layers (0.355 nm high) on a graphite surface. These atomic steps provide a much higher aspect ratio than standard AFM tips (radius 5-10nm) and hence can be used for the tip characterization. The image of a graphite step contains information about the shape of the lowest few nanometers of the tip. The width of the imaged step can be used as a measure for the resolution.

To test the results of the calibration method, a sample of hexacontane on graphite was used. As expected the lamellar structure of the sample with a periodicity of 7.5 nm could be imaged with sharp tips while with the blunter tips imaging of the lamellae was impossible.

CPP 15.5 Tue 18:15 Poster A

Impurity Spectroscopy at its Ultimate Limit: Relation between Bulk Spectrum and the Distributions of Individual Parameters of (Nearly) All Dopant Molecules in Solids — Andrei V. Naumov[1], Aleksey A. Gorshelev[1], Yury G. Vainer[1], •Lothar Kador[2], and Jürgen Köhler[2] — [1]Molecular Spectroscopy Department, 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

We recorded the fluorescence excitation spectra of a substantial fraction of all single chromophore molecules (hundreds of thousands and more) in solid bulk samples. The complete spectra and the spatial coordinates of all chromophores were stored for further analysis. In this way it is possible to study a bulk sample in a broad spectral region given by the inhomogeneous width of the electronic transition with ultimate sensitivity, combining excellent statistical accuracy and the capability of detecting rare events. From the raw data, the distributions of a number of parameters of the chromophore spectra were extracted, including the frequencies of the zero-phonon lines, their linewidths, and fluorescence count rates. Relationships between these distributions and the disorder of the matrix were established for the examples of two polycrystalline matrices of very different properties, n-hexadecane and o-dichlorobenzene, and the amorphous polymer polyisobutylene. Spatially inhomogeneous distributions of some parameters were found.

CPP 15.6 Tue 18:15 Poster A

Conceptual design for a new small angle X-ray scattering instrument at the Petra III extension — •Rainer Gehrke, Ulla Vainio, and Jan Perlich — Deutsches Elektronensynchrotron DESY, Notkestrasse 85, D-22603 Hamburg (Germany)

The storage ring DORIS III at DESY/Hamburg will stop operation at the end of 2012. A couple of experimental techniques which are presently not available at PETRA III have to be established at the new machine. Among these techniques are the various kinds of small angle X-ray scattering with moderately focused beams which are carried out at DORIS III beamlines A2, B1, and BW4 at present. In the frame of a PETRA III extension project a new versatile SAXS instrument is under planning which will allow performing SAXS in transmission and reflection geometry. It will feature a mini-undulator, a non-dispersive double crystal monochromator, horizontally and vertically focusing mirrors, and a maximum sample to detector distance of about 20 meters. The planned setup will also offer to utilize anomalous scattering in all possible scattering geometries.

The details of the components of the beamline layout (source, optics, experimental hutch) are discussed and ray tracing calculations are presented which allow estimating the beam properties in terms of beamsize, photon flux, etc.

CPP 15.7 Tue 18:15 Poster A

A sample holder for soft x-ray absorption spectroscopy of liquids in transmssion mode — •Simon Schreck, Gianina Gavrila, Christian Weniger, and Philippe Wernet — Institute for Methods and Instrumentation for Synchrotron Radiation Research, Helmholtz-Zentrum Berlin, Germany

Applying soft x-rays to liquids is challenging due to the incompatibility of the vacuum environment required for soft x-rays and the high vapor pressure of liquids. When recording soft x-ray absorption spectra in transmission mode, which is the most direct and efficient way, the strong attenuation of soft x-rays in matter calls for ultrathin samples.

Here we present a novel sample holder for soft x-ray absorption spectroscopy of liquids in transmission mode based on sample cells with x-ray transparent silicon nitride membranes. The sample holder allows for a reliable preparation of ultrathin liquid films with an adjustable thickness in the nm-μm range. This enables measurements of high quality x-ray absorption spectra of liquids in transmission mode, as will be shown for the example of liquid H2O, aqueous solutions of 3d-transition metal ions and alcohol-water mixtures. The fine structure of the x-ray absorption spectra is not affected by the sample thickness. No effects of the silicon nitride membranes were observed in the spectra. It is shown how an inhomogeneous thickness of the sample affects the spectra and how this can be avoided.

The measurements were performed at the synchrotron radiation source BESSYII at the Helmholtz-Zentrum Berlin.

CPP 15.8 Tue 18:15 Poster A

Combining UV-Vis and microGISAXS — •Roman Mannweiler[1], Matthias Schwartzkopf[1,2], Johannes F. H. Risch[1], Sebastian Bommel[1,3], Alke Meents[1], and Stephan V. Roth[1] — [1]Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, D-22607 Hamburg, Germany — [2]Universität Hamburg, Institut für Technische und Makromolekulare Chemie, Bundesstr. 45 20146 Hamburg, Germany — [3]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

Due to the immense technical development going hand in hand with a growing need for raw materials especially for metals, we must consider that our resources are finite. Therefore there is a growing need for alternative materials, which can easily be produced and have tailored properties at the same time which is one of the tremendous advantages of nanocomposites. In detail, polymer-metal nanocomposites can be designed by using different types of nano-particles and coating-procedures, so that they deliver many possibilities for different applications, like optical wirings in processing units or photovoltaic devices. Here, we restrict ourselves to determining the optical properties of such a nanocomposite by using UV-Vis-Spectroscopy. We present two applications examples, namely sputter-deposited gradient samples as well colloidal layer systems, to relate nanostructural changes with spectroscopic features.

CPP 15.9 Tue 18:15 Poster A

Soft x-ray emission spectroscopy on liquid jets - probing valence structure of solvents and solutes — •Kristjan Kunnus[1], Martin Beye[1], Alexander Föhlisch[1], Christian Kalus[1], Kerstin Kalus[1], Wilson Quevedo[1], Simon Schreck[1], Edlira Suljoti[1], Christian Weniger[1], Philippe Wernet[1], Sebastian Grübel[2], Ivan Rajkovic[2], Simone Techert[2], Franz Hennies[3], and Brian Kennedy[3] — [1]Helmholtz-Zentrum Berlin, Berlin, Germany — [2]Max-Planck-Institut für Biophysikalische Chemie, Göttingen, Germany — [3]MAX-lab, Lund, Sweden

We have developed an experimental set up which combines an in vacuum liquid jet with a soft x-ray emission spectrometer to enable resonant inelastic soft x-ray scattering (RIXS) measurements from liquids. RIXS is a powerful technique which enables to probe occupied and unoccupied electronic states with elemental and chemical selectivity. Advantages of using a liquid jet are continuous replenishment of the sample and absence of membranes to separate the liquid from the vacuum. These properties make the setup suitable for complementary usage at synchrotrons and x-ray free electron laser facilities. As example, RIXS L-edge spectra of K$_3$[Fe(CN)$_6$] and CrCl$_3$ aqueous solutions together with K-edge spectra of bulk water and alcohols are presented. These measurements were done at the BESSYII synchrotron radiation facility in Berlin, Germany.

CPP 15.10 Tue 18:15 Poster A

Space-resolved dynamic light scattering probing inhomogeneous dynamics in soft matter — •Sebastian Golde, Markus Franke, and Hans Joachim Schöpe — JoGu Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Germany

Dynamic light scattering (DLS) is the most powerful tool determining the dynamics in soft matter in a huge time interval of eleven decades. Using standard techniques the ensemble averaged dynamics can be determined in ergodic media. In nonergodic samples the time-averaged and the ensemble-averaged one differ. Special techniques have been developed (Interleaved sampling [1], Echo technique [2], multispeckle (MS) analysis [3]), measuring the intensity autocorrelation function (ICF) of many different coherent areas (speckles) simultaneously, in order to obtain ensemble averaged data. We here present a comparison of a new designed MS-DLS experiment with the Echo technique. In order to measure many speckles simultaneously we map the sample onto a fast CCD as a detector, which allows us to monitore the intensity of more than 500 speckles simultaneously and to connect each speckle with its origin scattering volume. Comparing the results from different method we obtain identical ensemble averaged results for coloidal hard sphere glasses. With the MS method we can achieve three decades shorter delay times than with the Echo method. Furthermore the MS setup allows us to measure time-resolved as well as space-resolved ICFs to probe differences in spatially separated subensembles. [1]Pr.Coll.Pol.Sci.100,121(1996) [2]Re.Sci.Inst. 75,2419(2004) [3]JCP 104,1758(1996)

CPP 15.11 Tue 18:15 Poster A

NMR spectroscopy in pulsed high magnetic fields — Benno Meier[1,2], •Jonas Kohlrautz[1], Jürgen Haase[1], Frederik Wolff-Fabris[2], Thomas Herrmannsdörfer[2], and Jochen Wosnitza[2] — [1]University of Leipzig, Faculty of Physics and Earth Science, Linnéstrasse 5, 04103 Leipzig, Germany — [2]Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany

We report on the first resolved nuclear magnetic resonance (NMR) measurement of different chemical shifts in pulsed magnetic fields at the Dresden High Magnetic Field Laboratory (Hochfeld-Magnetlabor Dresden). After having minimized the field inhomogeneity across our sample volume down to 35 ppm by reducing the sample dimensions to 0.5 mm in all directions, resolved ^{19}F spectra of a mixture of hexafluorobenzene and benzotrifluoride were observed, yielding a chemical shift difference of 100 ppm. The scaling of the NMR linewidth with the sample size indicates that the linewidth is determined by spatial variation of the applied field over the sample volume. Thus, it is expected that one can further increase the resolution by reducing the sample dimensions. The spectra are demodulated using our recently demonstrated full understanding of the time dependence of NMR signals in pulsed magnetic fields up to 62 Tesla.

CPP 15.12 Tue 18:15 Poster A

Applicability of local thermal analysis using heatable AFM probes with respect to environmental influences for monitoring polymer surface properties — •Martin Laher, Thomas Fischinger, and Sabine Hild — Institut für Polymerwisschaften, Johannes Kepler Universität Linz

Local thermal analysis (LTA) in the nanometer scale has nowadays become a commercial add-on for atomic force microscopes. Heatable cantilever probes with tip radii below 50 nm provide the possibility to perform LTA measurements at defined surface positions with nanometer resolution. On condition that an appropriate tip-temperature calibration has been conducted, phase transition temperatures can be measured. Modification processes like solvent treatment or plasma activation are proposed to change thermo-mechanical properties. In this study, LTA is used to investigated the influence of activation parameters like plasma power or treatment time in softening temperatures on a close to surface region. It has been shown that for time dependent effects like solvent evaporation from swollen polymer surface layers there is an influence of one LTA measurement on subsequent ones. Point arrays of measurements show a thermal influence of each LTA on the surrounding area of several microns which decreases resolution. Supplying additional thermal energy to the sample with an external heater reveals that LTA does not probe softening temperatures but rather the amount of thermal energy transferred. Force distance measurements of mechanical properties are compared to thermal LTA results.

CPP 15.13 Tue 18:15 Poster A

The Interaction of Carbon Dioxide with Water Molecules: DFT-based Path-Metadynamics — •Grégoire Gallet[1], Fabio Pietrucci[1], and Wanda Andreoni[1,2] — [1]Centre Européen de Calcul Atomique et Moléculaire, École Polytechnique Fédérale de Lausanne, Switzerland — [2]Institut de Théorie des Phénomènes Physiques, École Polytechnique Fédérale de Lausanne, Switzerland

We present an extensive study of the formation and dissociation of reactions $CO_2+nH_2O \leftrightarrows H_2CO_3+(n-1)H_2O$ in gas phase. We use both standard static approaches and path-metadynamics [1] to uncover the reaction mechanisms and to reconstruct the free energy surfaces. Our calculations are based on the pseudopotential/plane-wave implementation of the Kohn-Sham equations [2] and use several GGA and hybrid xc-functionals. Stringent validation tests of the computational methods were made and the performance of several xc-functionals was investigated. Excellent agreement was found among the different methods regarding the equilibrium and transition states configurations. Moreover, in spite of sizable differences in binding energies, all schemes agree in predicting the catalytic effect of water addition, also quantitatively. The role of entropy in determining the free energy barriers is critically investigated. [1] D. Branduardi, F.L. Gervasio and M. Parrinello; *J. Chem. Phys.*, **126**, 054103 (2007). [2] CPMD, *www.cpmd.org*; ©IBM Corp 1990-2012,©MPI für Festkörperforschung Stuttgart 1997-2001

CPP 15.14 Tue 18:15 Poster A

Electrical fine tuning of liquid crystal lasers — •Jürgen Schmidtke and Heinz-Siegfried Kitzerow — Department Chemie, Universität Paderborn, Germany

We demonstrate high-precision, continuous, electrical tuning of a photonic band-edge laser based on a dye-doped cholesteric liquid crystal. A micro-patterned array of electrodes creates an electric field perpendicular to the cholesteric helix, which distorts the chiral order of the liquid crystal, thus shifting the resonant band edge modes. This configuration allows for smooth tuning of the laser emission in a wavelength range of about 4 nm, using low voltages (of the order of 10 V).

CPP 15.15 Tue 18:15 Poster A

Revised self-consistent continuum solvation in electronic-structure calculations — Oliviero Andreussi[1], •Ismaila Dabo[2], and Nicola Marzari[1] — [1]Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne — [2]CERMICS, Project-team INRIA Micmac, Université Paris-Est

The solvation model proposed by Fattebert and Gygi [1] and Scherlis et al. [2] is reformulated, overcoming some of the numerical limitations encountered and extending its range of applicability. The resulting self-consistent continuum solvation (SCCS) [3] model provides a very effective and compact fit of computational and experimental data, whereby the static dielectric constant of the solvent and one parameter allow to fit the electrostatic energy provided by the PCM model with a mean absolute error of 0.3 kcal/mol on a set of 240 neutral solutes. Two parameters allow to fit experimental solvation energies on the same set with a mean absolute error of 1.3 kcal/mol. A detailed analysis of these results, broken down along different classes of chemical compounds, shows that several classes of organic compounds display very high accuracy, with solvation energies in error of 0.3-0.4 kcal/mol, whereby larger discrepancies are mostly limited to self-dissociating species and strong hydrogen-bond forming compounds.

[1] J. L. Fattebert and F. Gygi, J. Comput. Chem. 23, 662 (2002).

[2] D. A. Scherlis, J. L. Fattebert, F. Gygi, M. Cococcioni, and N. Marzari, J. Chem. Phys. 124, 074103 (2006).

[3] O. Andreussi, I. Dabo and N. Marzari, submitted to J. Chem. Phys.

CPP 15.16 Tue 18:15 Poster A

Generation of excited electron pulses by silicon–silicon oxide–platinum devices — •Michael Scheele and Detlef Diesing — Fakultät für Chemie, Universität Duisburg-Essen, 45117 Essen, Germany

Thin layer systems as the employed silicon–silicon oxide–platinum devices are used in studies of surface chemical reactions. In socalled chemicurrent measurements the tunneling current of the top electrode through the insulating oxide to the back electrode is monitored in the course of exothermic surface reactions. On the other hand one can push electrons of the back electrode to the top electrode by help of a bias voltage U. These electrons may induce surface reactions due to their intrinsic excess energy $e \cdot U$. This approach has barely been used yet. The pulsed voltage technique allows the injection of e.g. $3 \cdot 10^{12} e^-$ with a pulse voltage of 4 V for a pulse length of 1 ms. In a first experiment the hot electron induced heating of the top electrode (20 nm platinum) is characterized. The top electrode temperature is accessible simultaneously by measuring the resistivity of the top platinum film. One can thus discriminate between heating and excitation induced effects in surface chemical experiments. The possibility to desorb molecules or induce reactions by use of voltage pulses will provide a new kind of electrocatalyst.

CPP 15.17 Tue 18:15 Poster A

Field-cycling NMR based analysis of the damage structure in Ionic crystals irradiated with swift heavy ions irradiated with swift heavy ions — •Michael Ditter, Simon Quittek, and Franz Fujara — Institut für Festkörperphysik, TU Darmstadt

Radiation damage in ionic crystals such as lithium fluoride has been extensively studied in the past, however so far no heavy ion irradiated samples were examined with field-cycling (FC) NMR. In lithium fluoride the nuclear spin lattice relaxation time is decisively influenced by the presence of paramagnetic impurities and defects like F-centers, induced by swift heavy ion irradiation. Most of these defects are concentrated in a halo around the ion tracks. Besides defects created directly by the projectiles secondary radiation, originating during the stopping process inside the crystal, causes damage beyond the ion range. For the full examination of this effect a spatial resolution, as offered by one of our FC spectrometers, is desirable. The distribution of the defects is thought to be mainly responsible for the observed magnetic field dependence of the relaxation rate. Thus NMR relaxometry, especially field-cycling techniques, is a suitable tool to gather information about the structure of radiation damage. Additionally NMR spectroscopy can be used to detect the presence of molecular fluorine and lithium colloids in the damaged zones. Our results obtained by these methods will be presented.

CPP 15.18 Tue 18:15 Poster A

Improving the performance of liquid crystal lasers by electric fields — •Jürgen Schmidtke, Lu Lu, and Heinz-Siegfried Kitzerow — Department Chemie, Universität Paderborn, Germany

During the past decade, self-assembled photonic band edge lasers based on dye-doped cholesteric liquid crystals have attracted considerable interest as tunable, miniature light sources. We demonstrate that the lasing threshold and slope efficiency of a liquid crystal laser can be improved by application of an electric field: Using a dye-doped cholesteric liquid crystal with negative dielectric anisotropy as the DFB laser structure, emission characteristics improves with increasing ac electric field along the cholesteric helix. Possible reasons are a partial suppression of thermally driven director fluctuations, as well as a stabilization of the planar cholesteric texture against disturbances by the optical pumping process.

CPP 15.19 Tue 18:15 Poster A

Design and Characterization of a Gas Sensor System Consisting of a Poly(amide-imide) and Cryptophane-A Covered Optical Fiber — Carmen M. Gonzalez Henriquez[1], •Ulrich G. Volkmann[1], Marcelo Cisternas[1], Rosario Ortega[1], Mauricio Sarabia[1], Patrick Huber[1], and Alvaro Henriquez[2] — [1]Surface Lab — [2]Plasma and Optics Lab, Facultad de Física, Pontificia Universidad Católica de Chile, Chile

The principal innovation of this project is the design of a gas sensor based on the usage of a mixture between poly(amide-imide) oligomer [1] as matrix and cryptophane-A [2] covering an optical fiber. The optical behavior of this system was studied upon adsorption of different gases, typical of the decomposition of organic matter: CO2, N2, CH4 and H2. Using ellipsometry in a modified PCSA-null setup, we detect large changes in the optical polarization as a function of gas pressure or concentration.

[1] Carmen M. Gonzalez Henriquez et al. Structural symmetry breaking of silicon-containing poly(amide-imide) oligomers and its relation to electrical conductivity and Raman-active vibrations. *Polymer Int* **(2011)**, DOI: 10.1002/pi.3169.

[2] Suozhu Wu et al. Mode-filtered light methane gas sensor based on cryptophane A. *Analytica Chimica Acta* **(2009)**, 633 (2), 238-243.

C.M. Gonzalez Henriquez acknowledges a scholarship from VRI Nr. 10/2010 (PUC). Work supported by FONDECYT project Nr. 1100882.

CPP 16: Poster: Colloids and Complex Liquids

Time: Tuesday 18:15–20:45 Location: Poster A

CPP 16.1 Tue 18:15 Poster A

Directional locking of colloidal monolayers driven across quasiperiodic substrate potentials — •Thomas Bohlein and Clemens Bechinger — 2. Physikalisches Institut, Universität Stuttgart, Germany

Particles driven across an ordered potential energy surface may either follow the direction of the driving force or become entrained along any of the commensurate directions of the substrate. Such directional locking effects are of great technological relevance since they allow sorting of particles according to their size or refractive index. In recent numerical simulations it was predicted that kinetically locked-in states also occur on quasiperiodic potential landscapes which raises the question whether periodicity or long range order of the substrate is the essential ingredient for directional locking. Here we experimentally study the sliding behavior of a two dimensional colloidal monolayer interacting with quasiperiodic light induced substrate potentials. When the direction of the driving is varied with respect to the substrate, we find directional locking at angles corresponding to the symmetry axes of the underlying potential. On the locking steps the colloids exhibit a cooperative, kink-driven particle motion and assemble into dynamically ordered structures.

CPP 16.2 Tue 18:15 Poster A

Colloidal Epitaxy on Quasicrystalline Surfaces — •Sharan Devaiah, Thomas Bohlein, and Clemens Bechinger — 2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany

Colloidal epitaxy is a powerful technique for creating three-dimensional structures useful for applications such as optical filters, switches and photonic materials. During this process, colloidal particles slowly sediment onto a patterned surface which then results in a highly ordered structure. Thus far, this process has only been used to create periodic colloidal crystals. Here, we report on experiments where we attempt to employ this process on templates with quasiperiodic order which are perfectly ordered but not periodic. Our experiments give us simultaneous access to the real space information and the diffraction pattern, thus enabling us to investigate if and how the initial quasiperiodic order of the template proliferates in the vertical direction through the monolayers.

CPP 16.3 Tue 18:15 Poster A

Phase behavior of colloidal monolayers on one-dimensional periodic and quasiperiodic light fields — •Lamiss Zaidouny and Clemens Bechinger — 2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany

Phase transitions of colloidal monolayers on light-induced substrate potentials have been demonstrated to provide novel insights into the phase behavior of two-dimensional systems on patterned surfaces. Due to the interplay of repulsive interparticle forces and their interaction with the substrate, interesting structures will form which are also observed in atomic systems. Here, we study the phase transitions of charged colloidal particles on arrays composed of one-dimensional laser lines which are created by a scanned laser beam whose diameter is highly asymmetric by passing a cylindrical lens. This allows the creation of laser lines with periodic and quasi-periodic order. In addition, to revisit light-induced freezing and melting, we present first results on how colloidal monolayers form in the presence of one-dimensional periodic potentials

CPP 16.4 Tue 18:15 Poster A

Colloidal flow and transport in micro structured porous media — •Frank Wirner[1,2], Christian Scholz[1], and Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Max-Planck-Institut für Intelligente Systeme, Heisenbergstraße 3, 70569 Stuttgart, Germany

The understanding of transport and flow phenomena in porous media is important for many problems which arise in various fields of science and engineering, ranging from agricultural, biomedical, chemical and petroleum engineering to soil sciences. Although the literature on porous media has been growing rapidly over the last decades it is still unclear, how transport properties of liquids through porous materials can be related to their structure. We study transport and flow properties of fluids and colloidal suspensions in a quasi-2D microporous system, created using soft lithography, over a wide range of flow regimes. The colloids act as tracer particles and visualize the flow field. A camera system with a temporal resolution of 2 ms and a spatial resolution of 0.4 μm is used to analyze the particle trajectories. The porous structures are artificially designed and therefore the structural parameters like Minkowski functionals and pore size distributions are fully known and can be related to dynamical flow variables, such as permeability or dispersion coefficients.

CPP 16.5 Tue 18:15 Poster A

Shape dependence of active Brownian particles — •Felix Kümmel — Universität Stuttgart, Stuttgart, Germany

We recently introduced a new species of active Brownian particles whose active motion is due to the local demixing of a critical binary liquid mixture and can be easily tuned by illumination [1]. Here, we focus on the shape dependence of such active swimmers, which are prepared by soft lithography. For chiral swimmers, we observe circular trajectories whose orientation depends on their chirality. When such particles come close to a straight wall, there are two different kinds of interaction. In one case, the particle slides stable along the wall, while in the other case it is reflected. In addition, other shapes of swimmers are investigated.

[1] G. Volpe, I. Buttinoni, D. Vogt, H.J. Kümmerer, and C. Bechinger. Microswimmers in patterned environments. Soft Matter, (7):8810{8815, 2011.

CPP 16.6 Tue 18:15 Poster A

Neutronscattering on discotic liquid crystals in the bulk and in the nanoconfined state — •Christina Krause[1], Bernhard Frick[2], Reiner Zorn[3], and Andreas Schönhals[1] — [1]BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany — [2]Institut Laue-Langevin, 6 rue Jules Horowitz, BP. 156, 38042 Grenoble, France — [3]Research Centre Jülich, 52425 Juelich, Germany

Discotic liquid crystals (DLC) consist of a flat and rigid aromatic core substituted by flexible aliphatic chains. While the former is responsible for the pi-pi-stacking, the latter increases the solubility and gives rise to a rich thermotropic behavior. DLCs are self-assembled materials. The disc-shaped molecules organize into columns that further assemble into two-dimensional arrays with a hexagonal mesophase. The alkyl chains fill the intercolumnar space giving rise to a nanophase separated state. Triphenylene derivatives as model systems for DCLs were investigated by neutron scattering in the bulk and in the confined state where both the vibrational density of states as well as the molecular dynamics on a time scale of ca. 1 ns (elastic scans) were considered. The influence of both the structure (length of the aliphatic chains) and the confinement will be discussed in detail.

CPP 16.7 Tue 18:15 Poster A

Glassy dynamics in Pyrene-1,3,6,8-tetracarboxylic tetra(2-ethylhexyl)esther studied by Differential Alternating Current Chip Calorimetry and Dielectric Relaxation spectroscopy — •Christina Krause, Huajie Yin, and Andreas Schönhals — BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, D-12205 Berlin

The glassy dynamics of the discotic liquid crystal Pyrene-1,3,6,8-tetracarboxylic tetra(2-ethylhexyl)esther is investigated by a combination of Differential Alternating Current Chip Calorimetry and Dielectric Relaxation Spectroscopy. The temperature dependence of the dielectric relaxation rate in the low temperature range might be described by means of the Vogel-Fulcher-Tamann equation. A detailed analysis shows that the glassy dynamics changes in the vicinity of the phase transition temperature. To unravel a different aspect of the underlying processes Differential Alternating Current Chip Calorimetry is applied. Dielectric and calorimetric data show a good agreement. In the higher temperature limit charge transport is detected. Experiments on confined Pyrene-1,3,6,8-tetracarboxylic tetra(2-ethylhexyl)esther are carried out in the near future.

CPP 16.8 Tue 18:15 Poster A

Block Copolymer Agglomerates in a Nematic Liquid Crystal — •Thomas Müller[1], Wolfgang Schöpf[1], Ingo Rehberg[1], Robin Pettau[2], Klaus Kreger[2], and Hans-Werner Schmidt[2] — [1]Experimental Physics V, University of Bayreuth, 95440 Bayreuth — [2]Macromolecular Chemistry I, University of Bayreuth, 95440 Bayreuth

The suspension of colloidal particles in a nematic liquid crystal solvent can induce local disturbance of the director field. This effect is known from spherical particles like water droplets or gas bubbles which are injected into the liquid crystal host [1, 2]. We investigate a small amount of a side chain liquid crystal triblock copolymer in the nematic liquid crystal 5CB as solvent material. The middle block of the copolymer is 5CB-functionalized and therefore soluble in the anisotropic phase, whereas the non-soluble end blocks can aggregate due to microphase separation. If the resulting agglomerates are big enough, the director deformations in the surrounding birefringent area can be observed with a polarizing microscope. We study the optical properties of a thin layer of this side group liquid crystalline mixture between two glass plates and present a model for the director configuration around the agglomerates. [1] P. Poulin, D. A. Weitz, Phys. Rev. E, 57 (1), 1998; [2] C. Völtz, et al., Phys. Rev. Lett., 97, 227801, 2006

CPP 16.9 Tue 18:15 Poster A

Fluid-Fluid and Fluid-Solid transitions in the Kern-Frenkel model from Barker-Henderson thermodynamic perturbation theory — •Christoph Goegelein[1], Flavio Romano[2], Francesco Sciortino[3], and Achille Giacometti[4] — [1]MPI für Dynamik und Selbstorganisation, Goettingen — [2]Physical and Theoretical Chemistry Laboratory, Oxford University (UK) — [3]Dipartimento di Fisica and CNR-ISC, Sapienza Universita di Roma, Piazzale A. Moro 5, 00185 Roma, Italy — [4]Dipartimento di Scienze dei Materiali e Nanosistemi, Universita Ca' Foscari Venezia, Calle Larga S. Marta DD2137, I-30123 Venezia, Italy

We study the Kern-Frenkel model for patchy colloids using Barker-Henderson thermodynamic perturbation theory. The model describes a fluid where hard sphere particles are decorated with one patch, so that they interact via a square-well potential if they are sufficiently close one another, and if patches on each particle are properly aligned. Both the gas-liquid and fluid-solid phase coexistences are computed and contrasted against Monte-Carlo simulations results. We find that the perturbation theory describes rather accurately numerical simulations all the way from a fully covered square-well potential down to the Janus limit (half coverage). In the region where numerical data are not available (from Janus to hard-spheres), the method provides estimates of the location of the critical lines that could serve as a guideline for further efficient numerical work at these low coverages. A comparison with other techniques, such as integral equation theory, highlights the important aspect of this methodology in the present context.

CPP 16.10 Tue 18:15 Poster A

Dynamics in disconnected lamellar phases — •Stefan Wellert[1], Matthias Karg[2], Lukasz Szymanski[3], and Cosima Stubenrauch[3] — [1]TU Berlin, Str.d. 17.Juni 124, 10623 Berlin, Germany — [2]University of Bayreuth, Universitätsstrasse 30, 95440 Bayreuth, Germany — [3]University of Stuttgart, Pfaffenwaldring 35, 70569 Stuttgart, Germany

This contribution discusses the results of a neutron spin-echo (NSE) experiment addressing the dynamics in disconnected lamellar phases. (Pseudo)binary water-CiEj-type surfactant systems were investigated. The combination of a surfactant forming a continuous lamellar phase extending to low surfactant concentrations with a surfactant forming a lamellar phase only at high concentrations results in a disconnected lamellar phase. Regarding the stabilization of the lamellar phase in the dilute and the concentrated regime, respectively, it is known that the dilute lamellar phases, where the interlamellar distances are larger than the membrane thickness, are stabilized by membrane undulations. In the case of the concentrated lamellar phases, attractive van der Waals and repulsive steric forces are the stabilizing mechanisms. It was shown that the disconnection only takes place if the distance between two bilayers is similar to the thickness of the bilayers and it was argued that the disconnection is tuneable by the rigidity of the monolayer. In this combined small angle neutron scattering and NSE experiment we discuss the influence of the structure factor on the dynamics. By applying the theoretical approach of Zilman and Granek we determine the bending elasticity constants.

CPP 16.11 Tue 18:15 Poster A

Trapping colloids via critical Casimir forces — •Matthias Tröndle[1,2], Andrea Gambassi[3], Ludger Harnau[1,2], and Siegfried Dietrich[1,2] — [1]Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany — [2]Universität Stuttgart, Germany — [3]SISSA - International School for Advanced Studies and INFN, Trieste, Italy

Colloids opposite to substrates patterned with stripes of different chemical boundary conditions experience normal and lateral critical Casimir forces. Upon approaching the critical point of the solvent, this generates laterally confining potentials for the colloids. The strength of these trapping potentials is reversibly tunable by temperature changes. Experimental measurements for colloidal particles immersed in a binary liquid mixture of water and 2,6-lutidine close to the critical demixing point agree with the corresponding theoretical predictions [1,2]. It turns out that critical Casimir forces are a sensitive probe to the details of the geometry of the substrate pattern. A suitable choice of chemical stripes forming the pattern may even lead to *levitation* of colloids at a stable distance from the substrate due to the critical Casimir effect [3].

[1] M. Tröndle, O. Zvyagolskaya, A. Gambassi, D. Vogt, L. Harnau, C. Bechinger, and S. Dietrich, *Mol. Phys.* **109**, 1169 (2011). [2] M. Tröndle, S. Kondrat, A. Gambassi, L. Harnau, and S. Dietrich, *EPL* **88**, 40004 (2009). [4] M. Tröndle, S. Kondrat, A. Gambassi, L. Harnau, and S. Dietrich, *J. Chem. Phys.* **133**, 074702 (2010).

CPP 16.12 Tue 18:15 Poster A

Triphenylene-based discotic liquid crystals in bulk and confined to alumina oxide membranes — •Christina Krause, Huajie Yin, and Andreas Schönhals — BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin

Discotic liquid crystals consist of a stiff aromatic core surrounded by flexible aliphatic side chains. As the disc-shaped molecules of the core self-organize into hexagonal columnar arrays, the alkyl chains fill the space between the columns yielding a nanophase separated state. A series of triphenylene-based discotic liquid crystals (2,3,6,7,10,11-Hexakis[n-oxy]triphenylene (HATn, n=5,6,8,10) is investigated by means of Dielectric Relaxation Spectroscopy, Differential Scanning and Differential Alternating Current Chip Calorimetry. Nanoporous alumina membranes with different pores sizes are filled with the triphenylene derivatives to study the influence of confinement on the dynamics in these discotic liquid crystals by means of Dielectric Relaxation Spectroscopy.

CPP 16.13 Tue 18:15 Poster A

Elastic Properties of nematic phase - DFT and simulations of hard spherocylinders — •Ellen Fischermeier, René Wittmann, and Klaus Mecke — Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany

A fluid of hard spherocylinders is an ideal model system to study liquid crystals and to test density functional theories. Here we show results of a recent fundamental measure theory (FMT) generalized to arbitrarily shaped hard bodies [1]. This functional provides analytic expressions for the isotropic and nematic free energy as well as the Frank elastic coefficients of the nematic phase. However there is one free parameter in the functional which has to be adapted empirically. Therefore we carried out molecular dynamics simulations with a highly flexible and massively parallel rigid body framework [2]. The obtained numerical data is compared to the analytic results and we present the findings of both methods.

[1] H. Hansen-Goos and K. Mecke, Phys. Rev. Lett. **102**, 018302 (2009)

[2] Klaus Iglberger and Ulrich Rüde, Computer Science - Research and Development **23**, 159 (2009)

CPP 16.14 Tue 18:15 Poster A

Optical trapping of gold colloids — •Andreas Königer and Werner Köhler — Physikalisches Institut, Universität Bayreuth

Using a strongly focused laser beam to trap and manipulate single colloidal particles is a well known procedure in life science and micro rheology. We have extended this technique using a convergent laser beam, with its focus well above a thin sample layer, to be able to manipulate many colloids simultaneously. Operating with an inverted microscope we have shown, how sedimented gold colloids can be lifted against gravity and collected in an almost 2-dimensional cage by radiation forces that act against the osmotic pressure of the compressed colloidal gas. Once collected, the cloud of colloids can be manipulated in a number of ways. It can freely be moved to arbitrary positions, where e.g. specific chemical reactions could take place. By time-multiplexing of the laser beam it is even possible to split the cloud into subensembles, which can than be manipulated independently and later be recombined by contact free purely optical means. We present a detailed analysis of the particle dynamics in the convergent light field and compare it to experimental data.

CPP 16.15 Tue 18:15 Poster A

Transient cage forming in polymer solutions by hot gold colloids — •Florian Schwaiger and Werner Köhler — Physikalisches Institut, Universität Bayreuth, Germany

Utilizing laser heated gold colloids with a radius of 125 nm as nanoscopic heat sources, we investigated the concentration bleaching in binary polymer solutions of polystyrene and toluene due to the Soret effect. Laser irradiation causes a significant temperature rise $T \propto 1/r$ due to the high absorbance at their surface plasmon resonance around 532 nm. As a consequence of the strong nonlinear coupling of the local order parameter to the temperature gradient, it induces a complex concentration field $c(t, r, M_w, T(r))$. We analyze in detail the stationary temperature, concentration and viscosity profiles. Furthermore, we present experimental results both on the observation of the concentration field and on the diffusion of heated colloids within their self-created cage. We find increasing anomalous diffusion with increasing laser power represented by a negative minimum in the step correlation function of the random walk.

CPP 16.16 Tue 18:15 Poster A

Spontaneous emulsification of thermotropic liquid crystals in aqueous surfactant solutions — •Karthik Peddireddy, Pramoda Kumar, Shashi Thutupalli, Stephan Herminghaus, and Christian Bahr — Max-Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany

Thermotropic liquid crystals (LCs) are organic liquids which are usually not miscible with aqueous phases. The presence of surfactants enables the generation of LC-in-water and water-in-LC emulsions, provided that sufficient mechanical energy is added to the system; in that respect the LC/water systems behave just as numerous non-LC oil/water systems.

We have recently observed that some common LC compounds (such as, e. g., the 4-n-alkyl-4′-cyanobiphenyls) can undergo a *spontaneous* emulsification process, running without addition of mechanical energy, when brought in contact with aqueous surfactant solutions. The details of the process and the observed transient structures depend on the type of the LC phase: For nematic phases we observe the formation of aqueous droplets in the nematic bulk phase as well as nematic droplets in the aqueous bulk phase. For smectic phases, transient structures appear which resemble the myelin figures formed by lyotropic lamellar phases in contact with water. Polarizing microscopy and fluorescence microscopy studies are conducted in order to elucidate the mechanism of this possibly new type of spontaneous emulsification.

CPP 16.17 Tue 18:15 Poster A

Friction within single pairs of DNA grafted colloids as studied by optical tweezers — •Mahdy M. Elmahdy[1,2], Olaf Ueberschär[1], Carolin Wagner[1], Tim Stangner[1], Christof Gutsche[1], and Friedrich Kremer[1] — [1]Institute of Experimental Physics I, Leipzig University, Linnéstrasse 5, 04103, Leipzig, Germany — [2]Department of Physics, Mansoura University, Mansoura 35516, Egypt

Optical Tweezers are employed to study the transition from sliding to stick-slip friction between two DNA grafted (grafting density ~1000 molecules per particle, number of base pairs per grafted chain ~4000) colloids. The latter are moved with a relative velocity in respect to each other ranging between 50 nm/s up to 3 μm/s; one colloid is fixed to a micropipette while the other is held in the optical trap hence enabling one to determine and to separate the forces of interaction in the direction parallel and perpendicular to the motion. Further parameter to be varied is the salt (NaCl) concentration of the surrounding medium at pH 8.5. A transition from sliding to stick-slip friction is found and shown to be controlled by the product of interaction volume and interaction time.

CPP 16.18 Tue 18:15 Poster A

Investigation of confinenment induced oscillatory forces in nanoparticle-suspensions by CP-AFM — •Sebastian Schön, Yan Zeng, and Regine von Klitzing — Stranski-Laboratorium, Department of Chemistry, TU Berlin, Strasse des 17.Juni 124, D-10623 Berlin

Thin films of nanoparticles suspensions show a layered ordering in the vicinity of the confining surfaces, giving rise to oscillatory changes in density and force. These originate from the entropic excluded volume effect and indicate a break in the translational symmetry of the bulk system. The study of oscillatory forces therefore serves as a direct means to understand the interactions between colloids and control their stability.

Force measurements have been performed by Colloidal Probe Atomic Force Microscopy (CP-AFM), where the colloidal probe on the cantilever and the substrate act as confining surfaces. Forces can be extracted form the deflection signal of the cantilever and are normalized with the radius of the colloidal probe.

In previous investigations the influence of particles concentration, size and ionic strength of the suspensions has been studied. Using Small Angle X-Ray Scattering (SAXS) good agreement of the characteristic lengths between confinement and bulk was demonstrated.

Latest research focus on effect of surface potential of the nanoparticles on the oscillatory forces investigating different systems of silica nanoparticles and micelles.

CPP 16.19 Tue 18:15 Poster A

Critical Casimir torques acting on cylindrical colloids and Janus particles — •Marcel Labbé-Laurent[1,2], Matthias Tröndle[1,2], Ludger Harnau[1,2], and Siegfried Dietrich[1,2] — [1]Max-Planck-Institut für intelligente Systeme, Stuttgart, Germany — [2]Universität Stuttgart, Germany

Critical fluctuations in fluids give rise to forces acting on immersed colloidal particles. These Casimir-like forces are attractive or repulsive depending on the chemical surface properties. Self-assembly of colloids opposite to *structured* surfaces, induced by the critical Casimir effect, is observed experimentally for colloidal particles immersed in a critical water-2,6-lutidine mixture and is in agreement with theory [1]. Asymmetrical particles experience a critical Casimir torque in the presence of varying boundary conditions. The strength and the direction of the torque depend on the particle shape. Rod-like and disc-like particles exhibit different self-orientation. Similarly, *Janus*-particles are subject to critical Casimir torques and self-orientate, which may be useful in view of current research or applications.

[1] M. Tröndle, O. Zvyagolskaya, A. Gambassi, D. Vogt, L. Harnau, C. Bechinger, and S. Dietrich, *Mol. Phys.* **109**, 1169 (2011).

CPP 16.20 Tue 18:15 Poster A

Confocal Microscopy of Colloidal Hard Sphere and Charged Sphere Fluids and Crystals — •Achim Lederer and Hans Joachim Schöpe — Johannes Gutenberg University, Mainz, Germany

Monodisperse suspensions of colloidal spheres with known interaction are a terrific model system for testing predictions by statistical physics. Their typical length scales are accessible via optical methods like light scattering in reciprocal and microscopy in real space. Light scattering leads to ensemble averaged observables like structure factors in reciprocal space with a high statistical accuracy, while information about the local order and the local dynamic are very difficult to get. A state-of-the-art technique to gain information about the local parameters of a colloidal system is the Laser Scanning Confocal Microscope (LSCM) which takes 3D-videos from a sample. By this method, the structure and dynamics of a colloidal suspension can be observed on a single particle scale ([1], [2]). In this work we investigate colloidal model systems with hard sphere and charged sphere interaction in the fluid and crystalline regime using LSCM. We determine the structure of the colloidal fluid in the equilibrium state as well as in the metastable regime showing significant differences between these states increasing with increasing metastability.

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[2] A. D. Dinsmore et al., Appl. Opt. 40, 4152 (2001)

CPP 16.21 Tue 18:15 Poster A

Magneto-optical Technique for Detecting the Biaxial Nematic Liquid Crystal Phase — •Tanya Ostapenko[1], Cuiyu Zhang[2], Samuel Sprunt[1], Antal Jákli[2], and James Gleeson[1] — [1]Department of Physics, Kent State University, Kent, Ohio 44242, USA — [2]Chemical Physics Interdisciplinary Program and Liquid Crystal Institute, Kent State University, Kent, Ohio 44242, USA

The existence of the biaxial nematic liquid crystal phase (N_b) has been the subject of much discussion since it was first predicted [1]. The geometry of the liquid crystal mesogen is important and it is thought that banana-shaped, or bent-core, liquid crystals will have an N_b phase. Recently, there have been attempts to find a bent-core liquid crystal that exhibits this phase, but there have been many conflicting reports about whether the N_b phase has been positively identified. One reason for the discrepancy is that there is currently no way to rule out surface effects or anchoring transitions, both of which may give a false positive identification of a uniaxial-biaxial nematic transition. Optical techniques usually rely on a sample cell rubbing treatment to align the sample, but optical misidentification could occur if the material is in a tilted uniaxial phase, which appears the same as a homeotropically-aligned biaxial phase. We have developed a technique that uses a magnetic field to align the uniaxial director, thus widening its application to any bent-core nematic material.

[1] M.J. Freiser. *Phys. Rev. Lett.* **24**, 19, 1041-1043 (1970).

CPP 16.22 Tue 18:15 Poster A

Dynamic percolation in microemulsions based on anionic and nonionic surfactants

— •Andreas Bischof, Christina Lederle, Andreas Weber, Tinka Spehr, and Bernd Stühn — TU Darmstadt, Experimentelle Physik kondensierter Materie, Germany

We study structure and dynamics of water-in-oil microemulsions with a focus on dynamics percolation phenomenon. In order to do this, we use dielectric spectroscopy. Comparing microemulsions based on different surfactants, we see a significant change in the percolation behaviour. We compare water-in-oil microemulsions based on anionic (AOT: Dioctyl sodium sulfosuccinate) and nonionic (i.e. C12E4: Pentaethylene glycol monododecyl ether) surfactants. Both display the known phenomenon of percolation that manifests itself in a steep increase of conductivity changing composition or temperature. We focus on the droplet phase and the temperature dependent behaviour to estimate the percolation temperature Tp. The percolation transition is observed with increasing temperature for ionic surfactants and decreasing temperature for nonionic surfactants. Moreover in the case of nonionic surfactant based microemulsions we study the effect of addition of salts. We compare results from dielectric spectroscopy to structural findings by means of small angle x-ray scattering (SAXS).

CPP 16.23 Tue 18:15 Poster A

Interactions between PEG and non-ionic surfactant layers

— •Andreas Weber, Andreas Barz, Tinka Spehr, and Bernd Stühn — Experimentelle Physik kondensierter Materie, Technische Universität Darmstadt

The interactions between polymers and soft surfactant layers are subject of current research interest. One system to study these interactions are microemulsions, thermodynamic stable mixtures of a polar liquid and a non-polar liquid stabilized by a surfactant. Depending on the composition of the system, these microemulsions can form various structures. One of these structures is the droplet phase. There, droplets of one component are dispersed in a matrix of the other component. We examine the phase diagrams of water in oil droplets stabilized by a non-ionic surfactant ($C_{12}E_5$, $C_{12}E_4$) to characterize the initial system by small angle X-ray-scattering and light transmission experiments. We add the hydrophilic polymer PEG to the microemulsion to investigate the interactions between these polymers and the curved surfactant layer of the droplets: While scattering experiments provide information about the structure of the interface, dynamic light scattering and dielectric spectroscopy give results concerning the dynamics of the droplets and the interface. Furthermore, by changing temperature it is possible to force the initial system into a lamellar phase. We also examine the effect of adding polymer to those structures.

CPP 16.24 Tue 18:15 Poster A

Ferrocene-Pyridine Block Copolymers in Solution - Cylindrical Micelles in Methanol

— •Stephan Hillmann[1], Martin Kraska[1], Markus Gallei[2], Roland Klein[2], Matthias Rehahn[2], and Bernd Stühn[1] — [1]Experimentelle Physik kondensierter Materie, TU Darmstadt — [2]Ernst-Berl-Institut für Technische und Makromolekulare Chemie, TU Darmstadt

Ferrocene-containing polymers attract much attention because of their unique mechanical, (electro)chemical, (opto)electronical or magnetic properties [1]. We present structural investigations of the block copolymer poly(vinylferrocene-b-(2-vinylpyridine)) (PVFc-b-P2VP) [2] dissolved in methanol. Results from Small angle X-Ray scattering (SAXS) and polarized and depolarized dynamic light scattering (DLS) are combined leading to a detailed understanding of the structure in solution [3]. We found cylindrical micellar structures with different length to diameter ratios depending on the bulk volume fraction ϕ of PVFc in P2VP. Cylindrical diameters could be determined by DLS and SAXS. We applied different diffusion models to the DLS data in order to extract cylinder lengths and diameters. Both scattering methods support the image of a solution of isolated dissolved cylinders.

[1] G. R. Whittell, I. Manners, Adv. Mater. 2007, 19, 3439

[2] M. Gallei et al. Macromolecules, 2010, 43 (4), 1844-1854

[3] M. Kraska, S. Hillmann, M. Gallei, R. Klein, M. Rehahn, B. Stühn, *in preparation*

CPP 16.25 Tue 18:15 Poster A

Predicting the Soret coefficient in binary mixtures via an additiv model of the heats of transport

— •Florian Schock, Steffen Hartmann, and Werner Köhler — Physikalisches Institut, Universität Bayreuth

Diffusion in a binary mixture not only originates from a concentration but also from a temperature gradient. The so-called Soret coefficient, which is the ratio of thermal diffusion coefficient and mutual mass diffusion coefficient, can be expressed by non-equilibrium quantities - the heats of transport -, and a thermodynamic factor that can be obtained from equilibrium properties. We have measured the Soret coefficient of a large number of binary mixtures of organic solvents at least at three different concentrations. The thermodynamic factors have been determined from the group contribution method Modified UNIFAC (Dortmund). We have found an additive model for the heats of transport of equimolar mixtures. This allows to predict the Soret coefficients of all possible symmetric binary mixtures from the measurement of a single system. The procedure is exemplified for a series of alkanes in comparison with existing data for a large number of solvents.

CPP 16.26 Tue 18:15 Poster A

Rotational behavior of thermophoretic driven Janus particles at a hard wall.

— •Andreas Bregulla[1], Ralf Seidel[2], Michael Mertig[3], Klaus Kroy[4], and Frank Chichos[1] — [1]Molecular Nanophotonics Group, University Leipzig — [2]DNA Motors Group, University of Technology Dresden — [3]Physikalische Chemie, Technische Universität Dresden — [4]Soft Condensed Matter Theory Group, University Leipzig

Janus particles are particles with asymmetric surface properties of their two half spheres. Due to this asymmetry they become of large interest as building blocks for new self-organized structures or they provide new unique optical properties if one site of the sphere is coated by noble metal films. In the latter case of a metallic coating of one half, the metal can be used as optically driven heat source to generate an asymmetric temperature distribution around the particle. This asymmetric temperature distribution leads to a thermophoretically driven directed motion of the particle as recently demonstrated. The detailed mechanisms of this driven motion is,however, not clear. Especially the contributions of local charge distributions, field enhancements and the interaction with substrate is unknown. In this contribution we investigate the rotational motion of gold capped polystyrene spheres nears a boundary with help of darkfield imaging and demonstrate that the interaction with the surface leads to a restricted rotational motion.

CPP 16.27 Tue 18:15 Poster A

An ionic liquid electrospray source based on the epoxy SU-8

— •Katharina Huhn, Markus Piechotka, Torsten Henning, and Peter J Klar — I. Physikalisches Institut, JLU Gießen

In this work the feasibility of SU-8 capillaries for the application in an electrospray source was investigated. The interaction between the capillaries and the applied ionic liquids was examined in detail. Therefore we manufactured a test system consisting of three patterned layers: two layers of SU-8 as well as a metallic extraction electrode. The SU-8 layers were structured by means of photolithography whereas the extraction grid was grown by electroplating. The ionic liquid droplet formation was observed by micrograph imaging. Furthermore the influence of an electric potential between extraction electrode and ionic liquid was investigated.

CPP 16.28 Tue 18:15 Poster A

Comparison of time-dependent friction and diffusion coefficients of single blank and DNA-grafted colloids in dilute polymer solutions - Drag reduction by DNA-grafting beyond linear response?

— •Olaf Ueberschär, Carolin Wagner, Tim Stangner, Christof Gutsche, and Friedrich Kremer — Institut für Experimentelle Physik I, Universität Leipzig

Recently, we discovered that single DNA-grafted colloids under shear flow in dilute λ-DNA solutions experience a drag force that is significantly reduced compared to equally sized blank microspheres. The maximum extent of this drag reduction was found to amount to 60% compared to the λ-DNA-induced contribution on the drag on blank colloids. Based on previous theoretical work, we proposed an explanation of this effect by analyzing the differences in the Stokes flow field around the blank and grafted colloids. Now, we present new experimental and theoretical results that help to elucidate further the effects of polymer accumulation and depletion around single colloids in dilute polymer solutions under thermal equilibrium and non-equilibrium steady state conditions. Special emphasis is laid on the question whether or not these effects still take place in the linear response regime. For this, we compare the experimental data obtained with our optical tweezers setup and a fast free particle tracking measurements. The two major measurement approaches towards friction coefficients on a single particle level (drag forces in Stokes flow, free diffusion paths) are discussed in detail. Good quantitative agreement with pertinent theoretical predictions further supports our argumentation and conclusions.

CPP 16.29 Tue 18:15 Poster A

Formation and Observation of geometric defects in 2D colloidal systems. — •David Polster, Georg Maret, and Peter Keim — Department of Physics, University of Konstanz, D-78464 Konstanz, Germany

In two-dimensional systems topological defects always occur as dislocation, pairs of dislocation or disclinations. These defects appear already near kbT and distort the hexagonal symmetric of the 2D crystal, whereby, according to the Kosterlitz-Thouless-Halperin-Nelson-Young theory, melting in 2D proceed. On the other hand so called geometric defects as isolated point defects need a lot more energy to be created which can experimentally be done with an optical tweezer. We study the particle configurations and the displacement fields of several defects in a 2D system of paramagnetic colloidal particles which are sediment to a water/air-interface. By applying a magnetic field perpendicular to the interface the particles form a 2D crystal with hexagonal symmetry which can be manipulated with an optical tweezer. Thereby, we are interested as well in vacancies as in interstitials and their interaction. Furthermore we study the formation of defect strings by creating more than two defects of the same kind, which rearrange and form a string consisting of two dislocations and a number of vacancies or interstitials in between.

CPP 16.30 Tue 18:15 Poster A

Microrheology using Optical Tweezers — •Christof Gutsche, Olaf Ueberschär, Carolin Wagner, Tim Stangner, and Friedrich Kremer — Institute of Experimental Physics I, Leipzig University, Linnéstrasse 5, 04103, Leipzig, 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 flow resistance of single DNA-grafted colloids in different media [1,2], (ii) the flow resistance of one blank colloid in a polymer solution [3] and (iii) the effective hydrodynamic radius of single DNA-grafted colloids as measured by fast Brownian motion analysis [5].

[1] C. Gutsche, M. Salomo, Y.W. Kim, R.R. Netz and F. Kremer. Microfluidic Nanofluidic 2(5), 381 (2006) ; [2] Y.W. Kim, V. Lobaskin, C. Gutsche, F. Kremer, P. Pincus and R.R. Netz. Macromolecules 42, 3650 (2009); [3] C. Gutsche and F. Kremer, M. Krueger and M. Rauscher, R. Weeber and J. Harting. J. Chem. Phys. 129, 084902 (2008); [4] C. Gutsche et al. Phys. Rev. E 76, 031403 (2007); [5] O. Ueberschär et al. Polymer 52, 1829 (2011)

CPP 16.31 Tue 18:15 Poster A

Microfabrication of a 3D asymmetric flow profile for chiral separations — •Carina Vosskötter, Lukas Bogunovic, and Dario Anselmetti — Experimental Biophysics and Applied Nanoscience, Faculty of Physics, Bielefeld University, Bielefeld, Germany

Chiral molecules (enantiomers) are molecules with the same molecular formula that can be transformed into the respective other isomer only by mirroring. Even if enantiomers - except for their optical activity - yield identical physical properties, they can still have completely different biochemical effects with respect to the metabolism of living organisms. At the present time, industrially synthesized chiral drugs are separated as far as required so that 25 % of all them are administered as pure enantiomers.

We conceived an alternative selector-free and continuously working concept to separate chiral objects within a lab-on-a-chip device. We show that it is possible to separate (asymmetric) chiral micro-objects within an asymmetric micro flow profile with a yield of 85 %.

Furthermore this so far two-dimensional concept is expanded into full 3D by introducing a novel two-component assembly strategy for the microchip, that can allow for a complex surface modification protocol to break the symmetry in every relevant dimension.

CPP 16.32 Tue 18:15 Poster A

Electron spectroscopy study of the interaction of copper with [EMIm]Tf$_2$N under the influence of aerobic conditions — •André Zühlsdorff, Angela Ulbrich, Markus Reinmöller, Wichard J. D. Beenken, and Stefan Krischok — Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, PF 100565, 98684 Ilmenau, Germany

The interest of Cu/Ionic Liquid (IL) systems is motivated by the possibility to produce Cu nanoparticles as well as the great potential for catalytic processes. A detailed knowledge of the electronic structure of the Cu/IL system and the behaviour under environmental conditions is therefore important. Due to the low vapour pressure of ILs it is possible to analyse their properties under ultra high vacuum (UHV) conditions. In the present study copper was deposited onto [EMIm]Tf$_2$N by electron beam evaporation. Afterwards the influence of copper on the surface electronic structure of [EMIm]Tf$_2$N was investigated by X-ray photoelectron spectroscopy (XPS). An enrichment of copper at the edge of the liquid film was observed. The storage of the Cu/IL system under aerobic conditions for several days leads to a formation of Cu^{2+} species. Additionally, a modification of the near surface chemical composition was found and will be discussed. By comparing the copper containing IL with the neat [EMIm]Tf$_2$N a modification of the valence band structure was observed. The reconstruction of the photoelectron spectra by density functional theory (DFT) gives decent hints to the origin of these additional valence band structures.

CPP 16.33 Tue 18:15 Poster A

Efficiency boosting in application: Influence of the Poloxamer size on the phase behaviour of skin friendly microemulsions for decontamination — •Sebastian Höhn[1], Ralph Neubauer[1], Christoph Schulreich[1], André Richardt[2], and Thomas Hellweg[1] — [1]Phys. und Biophys. Chemie (PC III), Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany — [2]WIS Munster, ABC-Schutz, Humboldtstraße 100, 29633 Munster, Germany

Bicontinuous microemulsions exhibit sponge-like domain structures of oil and water separated by an enormous surfactant interface and are therefore excellent media for enzymatically catalysed reactions.

The addition of small portions of amphiphilic polymers can increase the efficiency of the surfactant, a phenomina known as the efficiency boosting effect. In this contribution the influence of the size of different commercially available triblock copolymers (Poloxamers) on two systems composed of sugar surfactant, alcohol, water, and oil is shown.

With the added block copolymers being a part of the amphiphilic interface, their effect on the size of the domains is of high interest. The results of small angle scattering methods (SAXS and SANS) for our model system based on n-decyl-β-D-maltoside ($C_{10}G_2$) and cyclohexane are compared with a technical system consisting of Simulsol SL55 ($C_{10-12}G_{1.3}$, Seppic) and Lanol99 (isononyl-isononate, Seppic). Here the influence of different Pluronic Polymers (BASF) on the phase diagram is presented.

CPP 16.34 Tue 18:15 Poster A

Analyzing polydispersity and deformation in confocal images of colloids — M. Roth, J. Wenzl, M. Franzmann, and •G. K. Auernhammer — MPI Polymer Research, Mainz, Germany

Confocal microscopy has been used to study the dynamical and structural properties of colloidal and granular matter. Three dimensional positions and translational motions of the constituent particles can be measured with high precision. Other quantities like forces or rotational motions, or the analysis of polydisperse samples, are harder to address.

Forces between particles in contact lead to deformations of the particles. For soft hollow spheres these deformations are large enough to be identified from confocal images. We present an extension to the algorithm by Crocker and Grier [1] to automatically extract the deformation particles (absoltute values and orientation) and thus forces on the particle. For this we use colloids that are only labelled in their surface. Convoluting the image of deformed hollow spheres with the expected image of the undeformed state leads to a correlation peak that carries the information about the deformation [2].

Additionally we show how to detect reliably the coordinates of polydisperse colloids in confocal images. We develop methods to reliable measure the position and extension of spherical particles. To illustrate the applicability of this algorithm we show the restructuring of colloidal aggregates under mechanical stress.

[1] J. C. Crocker and D. G. Grier, J. Coll. Int. Sci., **179**, 298 (1996).

[2] M. Roth, M. Franzmann, M. D'Acunzi, M. Kreiter, and G. K. Auernhammer, arXiv:1106.3623v1 [cond-mat.soft] (2011).

CPP 16.35 Tue 18:15 Poster A

Structure factor of model polydisperse ferrofluids with relatively weak interparticle interactions — •Ekaterina Krutikova[1], Sofia Kantorovich[1,2], and Alexey Ivanov[1] — [1]Ural Federal University, Lenin av 51, 620083, Ekaterinburg, Russia — [2]Institute for Computational Physics, Pfaffenwaldring 27, 70569 Stuttgart

Scattering measurements allow to obtain the so-called structure factor, which is, actually, the Fourier transform of the pair correlation function of the ferroparticle system. Thus, for correct processing of experimental data it is necessary to develop the theoretical model for the pair correlation function and structure factor. Here, we present a theory based on the diagram expansion of the pair particle potential, and molecular dynamics simulations for various polydisperse systems, and analyse the behaviour of the first peak of the structure factor, namely its height and width as a function of the ferrofluid granulometric composition.

CPP 16.36 Tue 18:15 Poster A

Magnetic properties of ferrofluids with shifted dipoles — •Taisia Prokopieva[1] and Sofia Kantorovich[1,2] — [1]Ural Federal University, Lenin av 51, 620083, Ekaterinburg, Russia — [2]Institute for Computational Physics, Pfaffenwaldring 27, 70569 Stuttgart, Germany

A statistical model has been developed to describe the magnetic properties of ferrofluids with shifted dipoles. Using the model, which is based on the "mean-field approach" [Ivanov A., Kuznetsova O., Physical Review E, 2001], we calculate the magnetization and initial susceptibility of the system of particles in which the dipole moment is shifted out from the center of mass towards the particle surface. Magnetic characteristics are calculated in the form of an expansion over the special potential of the interparticle interaction for shifted dipoles [Kantorovich S., Weeber R., Cerda J., Holm Ch., Soft Matter, 2011]. The influence of the relative shift of the magnetic moment (that is the ratio of the shift to the radius of the particle) on the magnetic properties of the system is demonstrated.

CPP 16.37 Tue 18:15 Poster A

Effective Confinement as Origin of the Equivalence of Kinetic Temperature and Fluctuation-Dissipation Ratio in a Dense Shear Driven Suspension — •Boris Lander[1], Udo Seifert[1], and Thomas Speck[2] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, Germany — [2]Institut für Theoretische Physik II, Heinrich-Heine-Universität Düsseldorf, Germany

In equilibrium, the fluctuation-dissipation theorem states that the ratio of a correlation function and the corresponding response function is time independent, its value - the fluctuation dissipation ratio (FDR) - is given by the thermal energy. Out of equilibrium, this time independence is not expected to hold anymore. However, studying response and velocity autocorrelation functions for a tagged particle in a shear driven colloidal suspension, we found a broad regime where this time independence still holds approximately to a very good degree. The approximately constant FDR is the kinetic temperature. We can now explain this a priori surprising observation, using the idea of an effective confinement in dense suspensions [1]. Exploiting a time-scale separation, we can derive an approximate form of the FDT involving the kinetic temperature as a constant scaling factor and an additive correction term. We show numerically that the latter is negligible in a broad parameter range. We also compare the system to a simple toy model, consisting of a single colloidal particle, trapped in a harmonic potential, subjected to shear flow. For this simple model, we also find a regime in which the FDR is approximately time-independent.

[1] B. Lander, U. Seifert, and T. Speck arXiv:1111.3589

CPP 16.38 Tue 18:15 Poster A

Non-equilibrium simulations of confined colloidal particles — •Tarlan Vezirov and Sabine H. L. Klapp — Institute of Theoretical Physics, Secr. EW 7-1, Technical University Berlin, Hardenbergstr. 36, D-10623 Berlin, Germany

We consider a confined non-equilibrium system of interacting colloidal particles driven by a planar shear flow. As a framework for solving the equation of motion,we employ the Molecular and Brownian Dynamics simulations. We investigate the impact of the shear flow and confinement on transport properties such as density profiles, mean-squared displacements and the diffusion coefficient.

CPP 16.39 Tue 18:15 Poster A

Time Dependent Excited State Solvation of a Polarity Probe — •Christoph Allolio and Daniel Sebastiani — Freie Universität Berlin Fachbereich Physik Arnimallee 14 14195 Berlin

The molecular probe *N*-methyl-6-quinolone (MQ) gives spectroscopic access to its local environment.[1] Using *ab-initio* molecular dynamics, we have simulated the excited state solvation of MQ[2] and the time evolution of its Stokes shift in aqueous solution. Results are in good agreement with experimental data obtained using femtosecond spectroscopy. The effect of electronic excitation is discussed in terms of the actual atomistic coupling to the surrounding hydrogen bond network and dipolar relaxation. Our understanding of the time dependent aqueous solvation around MQ is then used to investigate hydrogen bonding dynamics in complex biophysical systems available to experimentalists.[3]

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2 C. Allolio and D. Sebastiani, Phys. Chem. Chem. Phys., 13, 16395-16403. (**2011**)

3 Sajadi, M., Ajaj, Y., Ioffe, I., Weingärtner, H., Ernsting, N. P. Angew. Chem. Int. Ed., 49, 454-457. (**2010**)

CPP 16.40 Tue 18:15 Poster A

Percolation transition of colloids in confined geometry — •Helge Neitsch and Sabine H. L. Klapp — Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

We have performed grand canonical Monte-Carlo simulations to investigate the percolation transition of a system consisting of colloidal particles in the bulk as well as in a slit pore system, where the particles are confined by two plain, smooth and parallel walls. The colloidal interaction is simply modeled via a square well potential with a short range of attraction of 4% of the hard core diameter. The percolation transition is linked to interesting physical properties like colloidal gelation, conductivity or the connectivity of cavities within porous media. In agreement with a recent publication [1] our results lead to the finding, that the critical exponents of the bulk and of the confined system are deviating from those of the 2D or 3D random percolation class. We furthermore present results for the influence of the wall separation on the locus of the percolation threshold [paper in preparation].

[1] J. Skvor and I. Nezbeda, Mol. Phys. **109**, 133-139 (2011)

CPP 16.41 Tue 18:15 Poster A

On a field-induced vapor-liquid phase transition in dipolar monolayers — •Sebastian Jäger, Heiko Schmidle, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We investigate suspensions of colloidal dipolar particles in quasi-two-dimensional systems that are exposed to external rotating fields. If the fields rotate within the plane of the dipolar monolayer and are of suitable strength and frequency [1], they can cause the particles to self-assemble into two dimensional aggregates. In this talk, we relate the cluster aggregation process to a vapor-liquid phase transition and investigate the dynamic behavior of the dipolar particles when exposed to the rotating fields. To do this, we make use of Brownian (Langevin) dynamics simulations (with and without hydrodynamic interactions) and Monte-Carlo simulations [2, 3].

[1] S. Jäger and S. H. L. Klapp, Soft Matter 7, 6606 (2011).

[2] H. Schmidle and S. H. L. Klapp, J. Chem. Phys. 134, 114903 (2011).

[3] S. Jäger, H. Schmidle, and S. H. L. Klapp, in preparation.

CPP 16.42 Tue 18:15 Poster A

Colloidal crystals confined by walls: static and dynamic aspects of structural transitions caused by misfit — •Dorothea

Wilms, Peter Virnau, and Kurt Binder — Johannes Gutenberg Universität, Mainz

A two-dimensional colloidal crystal is studied under confinement of structured walls in one direction. Introducing a misfit by placing the walls closer together leads to a structural transition from n rows to (n-1) rows of crystalline particles and the development of soliton-staircases.

This system is investigated using Langevin Dynamics. We discovered an unusual mechanism of diffusion, where groups of particles make a collective circular movement.

The same system has been investigated under shear. Depending on the shear velocity, different effects were observed, ranging from the development of holes in the system to large parts of the crystal changing the orientation of their layers.

CPP 16.43 Tue 18:15 Poster A

Phase behavior of microemulsions with weak and strong surfactants — Harsha Paroor and •Doris Vollmer — MPI for Polymer Research, Mainz, Germany

Microemulsions are thermodynamically stable, isotropic mixtures of water, oil and surfactant. Depending on the temperature and concentration, surfactant molecules associate into a micellar, lamellar, hexagonal or sponge like bicontinous structure. To quantitatively predict the phase behavior we proposed a modified Helfrich equation describing the morphologies. It assumes that within a well-defined temperature interval two spontaneous curvatures coexist. To investigate the validity of this assumption we investigate the phase boundaries by various measurements. The spontaneous curvature is calculated from fitting the emulsification boundaries. Experimentally determined values for the phase transition temperatures and specific heat have been successfully fitted to the unified model.

CPP 16.44 Tue 18:15 Poster A

Disentangling Free-Energy and Diffusivity Contributions of Water Kinetics in Bulk and at Interfaces — •Yann von Hansen[1,2], Felix Sedlmeier[1], Liang Mengyu[1], Dominik Horinek[1], and Roland R. Netz[1,2] — [1]Physik Department, TU München — [2]Fachbereich Physik, FU Berlin

We use a recently developed method based on the Fokker-Planck equation [1] to disentangle the contributions of the free energy and diffusivity profiles on the local stochastic dynamics of single water molecules in bulk and at interfaces. Based on the trajectories of the separation between water molecule pairs from MD simulations, we investigate the bond breakage dynamics in bulk water. From the spectrum of mean first-passage times, the diffusivity profile along the separation coordinate is derived. The six-fold friction increase at small separations and the variations in the diffusivity profiles can be interpreted in terms of a dominant reaction path that involves additional orthogonal coordinates [2]. Using the same methodoly, we study the water kinetics at hydrophobic and hydrophilic substrates and solutes and obtain diffusivity profiles showing significant differences, which can be attributed to the presence of hydrogen bonds [3].

[1] M. Hinczewski et al., J. Chem. Phys. 132, 245103 (2010)
[2] Y. von Hansen et al., Phys. Rev. E 84, 051501 (2011)
[3] F. Sedlmeier et al., J. Stat. Phys. 145, 240-252 (2011)

CPP 16.45 Tue 18:15 Poster A

Fundamental measure density functional for the soft sphere erf-model — •Markus Burgis and Matthias Schmidt — Theoretische Physik II, Physikalisches Institut, Universitaet Bayreuth, D-95440 Bayreuth

As a generic model for soft colloids we consider a fluid of repulsive particles where the Mayer bond is a superposition of two error functions, which allows to interpolate between hard spheres and Gaussian cores. The corresponding pair interaction potential contains the colloidal size and the length scale over which the soft repulsion decays. We deconvolve the Mayer bond for general mixtures of such particles into single particle weight functions. Both the soft sphere weight functions and the Kierlik-Rosinberg scalar hard sphere weight functions follow from a set of coupled partial differential equations, where first derivatives with respect to the geometric model parameters are related to (multiple) application of the Laplace operator in position space. Rescaling the length scales in the weight functions allows to construct an accurate star approximation to the exact triangle diagram in the virial series. Corresponding scaling and exploiting isometric transformations of the weight functions leads to a fundamental measure free energy density functional for the pure fluid. Considering cases where the particle core is effectively impenetrable, we calculate the bulk fluid radial distribution function via the Ornstein-Zernike route. Comparison to results from our Monte Carlo simulations demonstrates over a broad range of densities that the theory accurately reproduces the loss of liquid structure upon increasing softness of the repulsion.

CPP 16.46 Tue 18:15 Poster A

DFT-reconstructed photoelectron spectra for metals in ionic liquids — •Markus Reinmöller, Angela Ulbrich, André Zühlsdorff, Stefan Krischok, Erich Runge, and Wichard J. D. Beenken — Institut für Physik und Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, Postfach 10 05 65, D-98684 Ilmenau

Metal atoms in ionic liquids (ILs) have gained interest for catalytic and electrochemical applications as well as an alternative route to generate nanostructures. Furthermore, alkali metal containing ILs may be utilized for storage of electrical energy. The combination of metals and an ionic liquid can be established in several ways: metal atoms may be deposited onto the IL, (electrochemically) dissolved in the IL or chemically bonded to the IL. In the present study copper and alkali metals like potassium are studied, which have been deposited (from vapour) onto the ionic liquid. To keep charge and spin balanced we have calculated clusters of ions and metal atoms by DFT and reconstructed the respective photoelectron spectra for core levels and valence band [1]. The theoretical spectra of the model systems have been compared to experimental photoelectron spectra (XPS, UPS).

[1] M. Reinmöller et al., Phys. Chem. Chem. Phys., 13 (2011) 19526.

CPP 17: Poster: Crystallisation, Nucleation and Self assembly

Time: Tuesday 18:15–20:15 Location: Poster A

CPP 17.1 Tue 18:15 Poster A

Stabilization of crystalline order in thin films of polyethylene close to a graphite substrate — •Ann-Kristin Löhmann, Thomas Henze, and Thomas Thurn-Albrecht — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Germany

The interface between a polymer melt and a crystalline surface plays an important role during crystal nucleation as well as during crystal growth. Thin polymer films on crystalline substrates can be considered as model systems. We present temperature dependent AFM measurements of thin polyethylene (LLDPE) films on graphite. Upon heating to the melting temperature the polymer film dewets leaving behind a thin ordered film of polyethylene showing the same lamellar structure as the semicrystalline film at lower temperatures. This ordered layer at the polymer-substrate interface is a few nanometres thick and stable at temperatures higher than the bulk melting point. For LLDPE-samples the ordered layer could be observed up to a temperature of 122°C, whereas the bulk melting point was 108°C. We speculate that this interfacial layer is responsible for heterogeneous nucleation on graphite and induces crystal growth of polyethylene perpendicular to the surface of the substrate.

CPP 17.2 Tue 18:15 Poster A

Microphase separation in the block copolymer PMMA-PBA synthesized by RAFT — •Stefanie Grünheit[1], Katharina Tietz[2], Alexander Rahn[1], Philipp Vana[2], and Konrad Samwer[1] — [1]1.Physikalisches Institut, Georg-August-Universität Göttingen — [2]Institut für Physikalische Chemie, Georg-August-Universität Göttingen

Block copolymers are known to separate into microphases with a rich variety of structures as lamellae or gyroids. Hence their phase diagrams are often complex and highly interesting to study. We want to develop a phase diagram for a polymer consisting of a soft (poly(butyl acrylate), PBA) block and a hard (poly(methyl methacrylate), PMMA) block.

Therefore polymers are synthesized by reversible addition-fragmentation chain transfer (RAFT) polymerization with different blocklength ratios as well as different overall chain lengths. Thermal analysis via thermogravimetric analysis (TGA) and dynamical mechanical analysis (DMA) are performed in order to get information about stability as well as glass temperatures and elastic properties. By means of X-ray scattering and atomic force microscopy (AFM) we want to examine the structural properties with regard to microphase separation.

The presence of two glass transitions as well as the observation of patterns in AFM-pictures suggest the occurence of microphase separated regions.

Financial support by the DFG SFB 937 is thankfully acknowledged.

CPP 17.3 Tue 18:15 Poster A

Effect of the crystalline α_c-process on the morphology of semi-crystalline polymers: a comparative SAXS study on poly-ϵ-caprolactone and polyethyleneoxide — •Anne Seidlitz, Albrecht Petzold, and Thomas Thurn-Albrecht — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle (Saale)

Semi-crystalline polymers can be classified into two different types, depending on the presence (α_c-mobile) or absence (crystal-fixed) of the α_c-Relaxation, which provides mobility to the chains in the crystals. Starting from a hypothesis made by Boyd, that all polymers with a high crystallinity are α_c-mobile while all polymers with a low crystallinity are crystal-fixed, we investigated the morphology of polyethyleneoxide (PEO) as a polymer with mobile crystalline chains and poly-ϵ-caprolactone as a polymer with fixed chains. We performed small angle x-ray scattering experiments at different molecular weights and crystallization temperatures. A simulation based on the paracrystalline model was developed to derive quantitative morphological information from the SAXS data. Clear differences between the structure of PCL and PEO were observed. For PCL the crystalline thickness d_c is well defined, while the amorphous thickness d_a displays a broad distribution. PEO shows a small, well defined d_a and a broad thickness distribution of the crystalline lamellae. Our interpretation is that the crystalline lamellae in PEO can reorganize during crystallization until a minimal d_a is established, while the morphology of PCL corresponds to a quenched state resulting directly from the crystal growth process.

CPP 17.4 Tue 18:15 Poster A

Shape-persistent linear, kinked, and cyclic oligo(phenylene-ethynylene-butadiynylene)s: self-assembled monolayers — •Stefan-Sven Jester, Alisa Idelson, Daniela Schmitz, Friederike Eberhagen, and Sigurd Höger — Rheinische Friedrich-Wilhelms-Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Self-assembled monolayers (SAMs) of shape-persistent rigid oligomers, particularly phenylene-ethynylene- butadiynylenes at the HOPG/TCB interface were studied by scanning tunneling microscopy (STM) with submolecular resolution. Substitution of the terminating acetylene functions of the linear oligomers with polar cyanopropyldimethylsilyl groups leads to 2D phase separation and defined rod-rod interactions, which determine the packing distances between the rigid rods. The results stimulated the connection of rigid rods via septiarylene clamp units. They covalently link two rigid rod units and define the intramolecular rod-rod distance that matches the alkoxy substituent chain lengths. The systems can be described as half-ring structures of two rigid rods connected via a rotatable joint unit. These acetylene-terminated half-ring structures were also oligomerized under Cu and Pd catalysis to yield defined acyclic and cyclic oligomers. Detailed STM studies decoded the molecular origin of the surface patterning of such systems. The dodecyloxy side chains are adsorbed along the HOPG main axes and, together with the alkoxy backbone angle, determine the adsorption direction of the adlayers. [1] S.-S. Jester, A. Idelson, D. Schmitz, F. Eberhagen, S. Höger, *Langmuir* **2011**, *27*, 8205.

CPP 17.5 Tue 18:15 Poster A

Shape-persistent macrocycles: 1D and 2D aggregation — Joscha Vollmeyer, •Stefan-Sven Jester, Friederike Eberhagen, and Sigurd Höger — Rheinische Friedrich-Wilhelms-Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

The aggregation of shape-persistent macrocycles towards one-dimensional supramolecular fibers is investigated. Atomic force microscopy investigation of individual supported fibers indicates lengths of up to several micrometers and diameters as low as 3 nm. The interaction of such highly anisotropic aggregates in cyclohexane leads microscopically to the formation of networks and macroscopically to a gel phase which was also characterized by means of differential scanning calorimetry and UV-vis spectrometry. Intraannular substitution of the macrocyclic cavity with an undecyldiether strand and a tetraethylene glycol strand significantly affect the aggregation behavior as compared to a macrocycle with hollow cavity. The same molecules form two-dimensional self-assembled monolayers at the solution/solid interface (1,2,4-trichlorobenzene/HOPG). However, all three shape-persistent macrocycles - independent of the intraannular substitutents - form adlayers with identical pattern structures. The results are of fundamental interest for the tailored design of sensor materials as well as functionalized adsorbate layers.

CPP 17.6 Tue 18:15 Poster A

Investigation of Flow-Induced Periodically Banded Single Crystals in Isotactic Polystyrene Thin Films — •Hui Zhang and Günter Reiter — Physikalisches Institut,Universität Freiburg,79104 Freiburg, Germany

Observation of crystallization in thin films by microcopy techniques offers possibility to reveal nature behind crystallization. Here, isotactic polystyrene (iPS) has been studied because of the low growth rate and high glass transition temperature, which make it convenient to control the crystallization process. We found in a certain temperature range the formation hexagonal concentric banded structures in single crystals grown in thin films, which named periodically banded single crystals. Using optical microscope, we determined the distance between neighboring bands which increased both with temperature and film thickness. Detailed studies by atomic force microscopy indicated the periodically banded structure is the result of regular variation on the number of layers in lamella stacks generated via screw dislocations which led to growth in the normal direction of the film. All lamellar layers were in registry, i.e. all chains oriented in the same direction. The mechanism responsible for the formation of this structure is discussed. To generate such periodic modulation in stack height, the depletion length ahead of the growing crystal must be significantly larger than the distance between two neighboring dislocations. Thus, crystal growth controlled by the diffusion process, which decides the number of molecule available at the growth front, can lead to the formation of regularly spaced stacks of lamellae.

CPP 17.7 Tue 18:15 Poster A

Crystallization kinetics of PET/MWCNT nanocomposites — •Andreas Wurm[1], Anja Herrmann[1], Andreas Korwitz[2], Doris Pospiech[2], and Christoph Schick[1] — [1]University of Rostock, Institute of Physics, Wismarsche Str. 43-45, 18057 Rostock — [2]Leibniz-Institut für Polymerforschung Dresden e.V., Dept. of Polymer Structures, Hohe Str. 6, 01069 Dresden

Isothermal and non-isothermal crystallization behavior of polymers can be investigated with traditional calorimeters often in a limited temperature region only. This results from the fast crystallization processes on optimal conditions, which appears in most polymers in a few seconds or less. The new chip-based Mettler Flash DSC 1 allows applying heating and cooling rates of several 1000 K/s, which enables for many polymers to follow crystallization in the whole temperature range between glass transition temperature and melting temperature. We applied the new chip calorimeter for the investigation of crystallization kinetics of PET/MWCNT nanocomposites under non-isothermal and isothermal conditions. The MWCNT act as nucleating agents for PET and speed up crystallization at high temperatures, where heterogeneous nucleation dominates, for about one order of magnitude. At low temperatures, where homogeneous nucleation in the polymer itself determines the rate, only small differences are observed, which leads to the conclusion, that polymer chain dynamics is not drastically changed due to presence of MWCNT in the PET matrix.

CPP 17.8 Tue 18:15 Poster A

Nucleation and Crystallization in Glassy Polymers (PCL, iPP) — Evgeny Zhuravlev[1], Daniela Mileva[2], René Androsch[2], and •Christoph Schick[1] — [1]Universität Rostock, Institut für Physik, Rostock, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Polymer Engineering Center of Engineering Sciences, Halle/Saale, Germany

Differential fast scanning chip calorimetry has been employed to study nucleation/ordering during annealing the glass of quenched polymers (PCL, iPP). Initially non-ordered samples were annealed below the glass transition temperature for different periods of time, and the change of structure during isothermal annealing was then analyzed by monitoring the exchange of latent heat on heating. Primary result of this work is the undoubted proof of homogeneous nucleation of ordering and mesophase formation in the glassy state. It is suggested that only local mobility of molecular segments is required to form small, ordered domains, and that the classical nucleation theory, which restricts nucleation of the crystallization/ordering process of polymers to temperatures between the equilibrium melting temperature and the glass transition temperature, needs modification.

CPP 17.9 Tue 18:15 Poster A

Heterogeneous and homogeneous crystal nucleation in colloidal hard-sphere like microgels at low metastabilities — •Markus Franke and Hans Joachim Schöpe — Johannes Gutenberg Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Germany

Crystal nucleation is dominated by heterogeneous nucleation in most cases, especially at low undercoolings (metastabilities, chemical potential differences) and for that reason heterogeneous nucleation on container walls or impurities is almost unavoidable. The hard sphere model system is the simplest model system showing a fluid crystal phase transition. Sterically stabilized colloidal particles in a refractive and density matching solvent provides such a hard sphere system for experimentalists. We studied the crystallization kinetics of homogeneous bulk as well as the heterogeneous wall crystallization within the fluid crystal coexistence region. Parameters characterizing the crystallization process (induction times, growth coefficients, nucleation rate densities,...) were determined by using time resolved static light scattering and Bragg microscopy. By performing further analysis according to classical nucleation theory we can show that wall crystallization is induced by complete wetting of the cell walls with crystalline layers leading to a vanishing nucleation barrier.

CPP 17.10 Tue 18:15 Poster A

Polymer induced changes of the crystallization scenario in suspensions of hard sphere like microgels — Richard Beyer, Sara Iacopini, Thomas Palberg, and •Hans-Joachim Schöpe — Institut für Physik, Johannes Gutenberg Universität, Mainz, Germany

We investigated the crystallization scenario of hard sphere like Polystyrene microgels suspended in the good solvent 2-Ethylnaphtalene using time resolved Bragg scattering. The slightly polydisperse samples were prepared at the melting volume fraction of the polymer free system around 0.55. For the polymer free samples we obtained polycrystalline solids via the two-step crystallization scenario known from hard sphere suspensions with little competition of wall crystal formation. Addition of non-adsorbing low molecular weight Polystyrene polymer leads to a considerably slowed crystal growth. Further we observed a delay of precursor to crystal conversion for the bulk particles while the induction times for wall nucleation are reduced. The increased polymer concentration thus shifts the balance between the two crystallization pathways and the relative amount of wall based crystals can be tuned.

CPP 17.11 Tue 18:15 Poster A

Protein crystallization in the presence of di- and trivalent metal ions — •Andrea Sauter[1], Georg Zocher[2], Fajun Zhang[1], Thilo Stehle[2,3], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Germany — [2]Interfaculty Institute of Biochemistry, Universität Tübingen, Germany — [3]Department of Pediatrics, Vanderbilt University, Nashville, USA

Structure determination of proteins requires high-quality single crystals. Our previous studies concerning reentrant condensation (RC) of proteins upon adding trivalent salts have opened up a way to a universal phenomenon that can be used to tune protein interactions and thus optimize protein crystallization [1,2]. RC is caused by ion binding at the protein surface and thus an effective charge inversion. We now investigated how globular proteins behave upon using divalent metal salts. A phase behaviour similar to RC is found for bovine β-lactoglobulin (BLG) with $CdCl_2$ or $ZnCl_2$. Zeta potential measurements show a charge inversion of the protein. However, no such behaviour could be observed for other proteins by adding divalent salts, indicating the specificity of BLG. We present the growth of BLG crystals using trivalent [3] or divalent ions and their structure determined by X-ray diffraction. The positions of the metal cations that bridge acidic side chains from neighbouring protein subunits were compared for different salts. Using BLG as a model system, the role of the di- and trivalent metal ions in protein crystallization is discussed. [1] F. Zhang et al., PRL, 101, 2008, 148101; [2] F. Zhang et al., Proteins, 78, 2010, 3450-3457; [3] F. Zhang et al., J. Appl. Cryst., 44, 2011, 755-762.

CPP 17.12 Tue 18:15 Poster A

Low temperature sol-gel synthesis of polymer/titania hybrid films based on custom made poly(3-alkoxy thiophene) — •Martin A. Niedermeier[1], Monika Rawolle[1], Phillip Lellig[2], Volker Körstgens[1], Eva M. Herzig[1], Adeline Buffet[3], Stephan V. Roth[3], Jochen S. Gutmann[4], Thomas Fröschl[5], Nicola Hüsing[5], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Max-Planck-Institut für Polymerforschung, 55128 Mainz, Germany — [3]HASYLAB at DESY, 22603 Hamburg, Germany — [4]Universität Duisburg-Essen, Institut für Physikalische Chemie, 45141 Essen, Germany — [5]Universität, Salzburg, FB Materialforschung und Physik, 5020 Salzburg, Austria

A low temperature route to directly obtain polymer/titania hybrid films is presented. For this, a poly(3-alkoxy thiophene) is synthesized and used in a sol-gel process together with an ethylene glycol modified titanate (EGMT), as the titania precursor. Atomic force microscopy and scanning electron microscopy reveals that the poly(3-alkoxy thiophene) acts as the structure directing agent for the titania matrix and still maintains a high degree of crystallinity, as shown with grazing incidence wide angle X-ray scattering. UV/Vis measurements show a similar absorption behavior to P3HT with an absorption maximum around 500 nm and the typical UV absorption behavior of rutile titania.

CPP 17.13 Tue 18:15 Poster A

Manipulating crystallization by seed induced heterogeneous nucleation — •Andreas Engelbrecht and Hans Joachim Schöpe — Johannes Gutenberg-Universität, Mainz, Germany

Most solids consist of crystals and their material properties are highly controlled by the crystallization kinetics. Controlling crystal nucleation and growth is of great interest in condensed matter physics and material science. Container walls and impurities are almost omnipresent making heterogeneous nucleation the dominant process in many cases biasing the material microstructure. We here present a crystallization kinetics study in a colloidal model system of charged spheres adding nucleation seeds analog to inoculation in metallic systems.

We performed video microscopy of the crystallization process observing nucleation and growth of both homogeneously nucleated and seed induced crystals. While single crystals form by homogeneous nucleation, multi domain crystals nucleate on seeds appearing like bloomy flowers. We are able to extract time resolved nucleation rate densities, crystal size distributions and induction times for different seed concentrations. We see homogeneously nucleated crystals compete with those induced by the seeds. Hence crystallization kinetics and therefore also the arising microstructure can be tuned with the amount of added seeds.

CPP 17.14 Tue 18:15 Poster A

Strain-induced nucleation for establishing highly oriented iPP — •Konrad Schneider — Leibniz-Institut für Polymerforschung Dresden, Germany

The mechanical properties of semi-crystalline materials are mainly determined by the morphology of the material, especially the crystalline phase. This can be controlled in a wide range by nucleating agents. By stretching of partially crystallized material the crystallite orientation of the subsequent crystallized phase can be influenced in a wide range. By simultaneous WAXS (wide angle x-ray scattering) during drawing and crystallization the built-up of the final structures can be followed. It will be shown, how which structural variability is possible by this procedure.

CPP 17.15 Tue 18:15 Poster A

Opal-like Crystals: Structural Analysis by Small Angle Neutron Scattering — •Parvin Sharifi Rajabi, Mulda Muldarisnur, and Frank Marlow — Max-Planck-Institut für Kohlenforschung, Mülheim (Ruhr), Germany

Spherical building blocks ordered in a close-packed fcc arrangement form opal-like structures. They are interesting photonic crystals. Self-assembly is a direct and cheap approach for the opal fabrication but mostly, it results in structures with many defects. The photonic properties of these structures are highly sensitive to the structural imperfection. Characterization by different diffraction approaches can resolve the details of the structure.

Opals and inverse opals were fabricated by capillary deposition method [1]. They were characterized optically, by SEM and mostly by SANS. The SANS data were analyzed in respect to structural imperfections and lattice deformations. The preliminary interpretation was significantly extended [2].

[1] H. L. Li, W. Dong, H. J. Bongard, F. Marlow, J. Phys. Chem. B 2005, 109, 9939.

[2] F. Marlow, M. Muldarisnur, P. Sharifi, H. Zabel, Phys. Rev. B 2011, 84, 073401.

CPP 17.16 Tue 18:15 Poster A

From atoms to layer: growth kinetics during sputter deposition observed via in-situ GISAXS

— •Matthias Schwartzkopf[1], Mottakin M. Abul Kashem[1], Gunthard Benecke[2], Adeline Buffet[1], Denise Erb[1], Berit Heidmann[1], Gerd Herzog[1], Volker Körstgens[3], Ezzeldin Metwalli[3], Jan Perlich[1], André Rothkirch[1], Kai Schlage[1], Peter Müller-Buschbaum[3], Ralf Röhlsberger[1], Rainer Gehrke[1], and Stephan V. Roth[1] — [1]DESY, Notkestr. 85, D-22607 Hamburg — [2]MPIKG, Dep. Biomat., Am Mühlenberg 1, D-14424 Potsdam-Golm — [3]TU München, Physik Department E13, James-Franck-Str. 1, D-85748 Garching

For an efficient and controllable production of active nanostructured surfaces, sputter deposition plays a very important role in industrial processing [1]. In order to tune the unique size-dependent optoelectronic and catalytic properties of gold clusters, it is mandatory to know, how the growth kinetics influences the metal film morphology during sputter deposition. We therefore investigate in-situ growth kinetics of gold during sputter deposition by grazing incidence small-angle-X-ray scattering (GISAXS). The high time resolution allows determining the growth kinetics of the initial nucleation and the subsequent 2D self-assembly of clusters at industrial deposition rates. The temporal evolution of the structural parameters reveals four general stages of gold cluster growth. We show that each stage is characterized by a predominant surface process and its intrinsic kinetics.

[1] Faupel et al., Adv. Eng. Mat. 12, 1177 (2010)

CPP 17.17 Tue 18:15 Poster A

Monodisperse polystyrene@vinyl-SiO2 core-shell particles and hollow SiO2 spheres for photonic crystals fabrication

— •Tian-Song Deng and Frank Marlow — Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr, Germany

SiO2-coated particles have been attracted much attention in recent years, since these core-shell particles have potential applications as chemical micro containers and colloidal crystals, and especially photonic crystals. In this paper a method of preparing highly monodisperse core-shell particles and hollow spheres is described. Both kinds of particles are very useful building-blocks for colloidal crystals. The key of the method is the use of vinyltrimethoxysilane as a precursor for the shells which are obtained by direct growth of vinyl-SiO2 on negatively charged PS template particles. This method delivers a tunable shell thickness (between 10 nm and 170 nm) combined with a very low polydispersity (smaller than 3%) and no aggregation of the obtained particles. Furthermore, the core-shell particles could be converted into hollow SiO2 spheres by removing the PS cores in a calcination process. Both, the PS@vinyl-SiO2 particles and the hollow SiO2 spheres can be self-assembled into colloidal crystals using their suspensions which are highly monodisperse and aggregation-free. The synthesis method might be extended for coating uniform organo-SiO2 shells on different kinds of core materials. In addition, the use of other organo-oxide precursors could lead to new hollow oxide particles useful for colloidal crystal formation.

CPP 17.18 Tue 18:15 Poster A

Universality in block copolymers: a corresponding states hypothesis

— •Jens Glaser, Jian Qin, Pavani Medapuram, and David Morse — Dept. of Chemical Engineering and Materials Science, University of Minnesota, 421 Washington Ave SE, Minneapolis, MN 55455, USA

Phase behavior and fluctuations of very long block copolymers are well described by self-consistent field theory, and by the random-phase (RPA) approximation for concentration fluctuations. The SCF / RPA predicts behavior that depends on only a few dimensionless parameters. More sophisticated coarse-grained theories instead suggest an extended form of this principle of corresponding states, in which the behavior is predicted to depend on one additional parameter, the independent degree of polymerization $\bar{N}$. We are testing this prediction by comparing extensive computer simulations of several different coarse-grained simulation models of AB diblock copolymer melts. We utilize a novel simulation methodology based on graphical processing unit (GPU) accelerated hybrid molecular dynamics / Monte Carlo replica exchange simulations on a cluster of many GPUs. We present data for off-lattice models with soft- and hard-core non-bonded interactions, and a lattice model, comparing simulations of different models that are designed to have matched values of $\bar{N}$. The results provide extremely strong evidence for the corresponding states hypothesis, which is found to remain accurate even for chains that are much too short to be accurately described by SCFT or the RPA.

CPP 17.19 Tue 18:15 Poster A

IR spectroscopic studies on SiO condensation

— •Steffen Wetzel and Annemarie Pucci — Kirchhoff-Institut für Physik, INF 227, 69121 Heidelberg

Silicon oxides used to be relevant as gate oxides in microelectronics and are of great importance in astronomy as building blocks of silicates, the most abundant minerals in space. The IR spectral feature of the Si-O stretching vibration strongly depends on the chemical composition and on the formation conditions. We studied the growth of thermally evaporated SiO on clean Si(111)7x7 at room temperature and found a strong shift of the resonance frequency for the first stage of film growth indicating the formation of an $\mathrm{SiO_x}$ $(0 \leq x \leq 1)$ interlayer. Condensation experiments at substrate temperatures between 40 K and 470 K reveal as well a clear shift of the resonance frequency, indicating gradual disproportination of SiO into Si and SiO_2 for the higher temperatures. Both effects will be discussed in detail and be presented along with details on the experimental setup.

CPP 17.20 Tue 18:15 Poster A

Nucleation and growth of large scale ordered structures in highly swollen thin-films of Poly-γ-benzyl-L-glutamate (PBLG)

— •Kaiwan Jahanshahi[1], Ioan Botiz[1,2], and Günter Reiter[1,2] — [1]Institute of Physics, University of Freiburg — [2]Freiburg Research Institute of Advanced Studies (FRIAS)

In the α-helical confirmation, the PBLG molecule exhibits chirality and a huge electrical dipole moment making it capable to form liquid crystal, fibrils and even large scales of ordered structures. The mechanisms governing these structure formations are still poorly understood which motivated our experimental study about PBLG assemblies obtained by solvent annealing of spin coated thin films. By controlling the physical parameters like polymer concentration with respect to the solubility limit (below which no ordered structures can nucleate), and also adding a non-solvent to the system, we can precisely control the nucleation density and the growth rate of large scale ordered structures as well as their shape and size in three dimensions. Consequently we could study the kinetics of growth process of Poly(γ-benzyl-L-glutamate) molecules in such systems and define time dependence of the size of the ordered structures as well as the effect of solvent/non-solvent ratio on the nucleation density of such structures.

CPP 17.21 Tue 18:15 Poster A

The Effect of Surface Affinity on the Morphology of Double Crystalline Co-Oligomer Thin Films

— •Robert Schulze, Thomas F. Keller, and Klaus D. Jandt — Institute of Materials Science and Technology, Friedrich-Schiller-University Jena, Germany

The lamellar morphology of double crystalline co-oligomers in the bulk was recently attributed to a stacking of extended or folded chains.

Thus, the aim of the present study was to show that the lamellar morphology of extended chains of a double crystalline co-oligomer can be used to create amphiphilic nanopatterns on surfaces.

Therefore we analyzed polyethylene-block-poly(ethylene oxide) co-oligomer thin films onto chemically different substrates by atomic force microscopy.

After drop-casting from dilute solution we observed quantized values of the film thickness that correspond to multiple integers of the theoretically extended chain length. On neutral surfaces, annealing leads to perpendicular lamellae, where the lamellar thickness resembles the theoretical extended chain length, whereas on hydrophilic and hydrophobic surfaces residual thin films possess no defined lamellar surface structure.

These observations can be explained by assuming that the formation of thin film morphology is dominated by the crystallization of extended chains under the influence of the surface affinity. On neutral surfaces, annealing facilitates a chain rotation from perpendicular to parallel, therefore enabling the formation of a lateral lamellar surface morphology with potential applications, as e.g. in the biomedical field.

CPP 18: Organic semiconductors I

Time: Wednesday 9:30–11:00 Location: C 130

CPP 18.1 Wed 9:30 C 130

Solvent induced morphology in polymer-based systems for organic photovoltaics — Matthias A. Ruderer[1], Shuai Guo[1], Robert Meier[1], Hsin-Ying Chiang[1], Volker Körstgens[1], Jan Perlich[2], Stephan V. Roth[2], and •Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany

In this investigation we probe the influence of the used solvent on the morphology formation of polymer-based bulk heterojunction systems for photovoltaic applications. Films are spin coated from different solvents. We chose the bulk heterojunction system consisting of the conjugated polymer P3HT (poly(3-hexylthiophene-2,5-diyl)) and the methano fullerene PCBM. Both components fit very well concerning their electronic behaviors and this combination is probably the best investigated system in organic photovoltaics so far. Besides imaging methods such as atomic force microscopy (AFM), the advanced scattering techniques X-ray reflectivity and grazing incidence small and wide angle X-ray scattering (GISAXS and GIWAXS) reveal a full understanding of the inner film structure on molecular to mesoscopic length scales. In combination with topography imaging we are able to reconstruct schematic morphologies from the scattering experiments for the films made from the different solvents. Depending on the solvent, enrichment layers at the interfaces as well as varying structural length scales inside the active layer are found [Adv. Funct. Mater. 21, 3382-3391 (2011)].

CPP 18.2 Wed 9:45 C 130

Influence of aggregation on the performance of all-polymer solar cells containing low-bandgap naphthalenediimide-copolymers. — •Marcel Schubert[1], Daniel Dolfen[2], Johannes Frisch[3], Steffen Roland[1], Robert Steyrleuthner[1], Burkhard Stiller[1], Zhihua Chen[4], Ullrich Scherf[2], Norbert Koch[3], Antonio Facchetti[4], and Dieter Neher[1] — [1]University of Potsdam, Germany — [2]University of Wuppertal, Germany — [3]Humboldt University Berlin, Germany — [4]Polyera Corporation, USA

Naphthalene-diimide (NDI) or perylene-diimide (PDI) containing copolymers are promising alternatives for replacing fullerenes as the electron-accepting phase in organic solar cells. So far, the power conversion efficiencies (PCEs) of all-polymer solar cells comprising NDI/PDI-based copolymers and regio-regular poly(3-hexylthiophene) (P3HT) remained below 1%. It was proposed that the NDI/PDI-copolymers exhibit a strong tendency to aggregate, which promotes long range phase separation and unfavourable nanomorphologies.

Our studies of the optical properties of such copolymers in different solvents reveal a strong tendency to pre-aggregate. This pre-aggregation could be fully suppressed by adding suitable high boiling point solvents. Solar cells prepared from these solvent mixtures showed PCEs of up to 1.4% and high fill factors of up to 70%, which are among the highest reported values for polymer-polymer blends. Finally, SNOM and AFM measurements in combination with optical absorption studies reveal a surprising anticorrelation between the degree of chain aggregation and the photovoltaic device performance.

CPP 18.3 Wed 10:00 C 130

Does conjugation help exciton dissociation? A study on poly(p-phenylene)s in planar heterojunctions with C_{60} or TNF — •Christian Schwarz[1], Heinz Bässler[1], Irene Bauer[1], Jan-Moritz Koenen[2], Eduard Preis[2], Ullrich Scherf[2], and Anna Köhler[1] — [1]Experimental Physics II, University of Bayreuth — [2]Macromolecular Chemistry, Bergische Universität Wuppertal

We report the field-assisted photocurrent generation in organic bilayer diodes with different poly(p-phenylene)s as donors and C_{60} or TNF as acceptor. The polymers differ regarding their torsional degree of freedom and concomitantly regarding their conjugation length and energetic disorder. We find the photocurrent yield to saturate around 100 % at fields between $5 \cdot 10^4 \frac{V}{cm}$ to $10^6 \frac{V}{cm}$. The saturation field required scales with the optical gap, implying that conjugation and energetic order is of crucial importance for the yield. We conclude that the rate limiting step for photogeneration is the formation of a loosely bound electron-hole pair that can either be collected by a moderate field or relax back to a tightly bound electron-hole pair.

CPP 18.4 Wed 10:15 C 130

Charge Transfer in Polymer:PC$_{60}$BM:PC$_{70}$BM triple Blends: Which Fullerene gets the Electron? — •Andreas Sperlich[1], Johannes Römer[1], Hannes Kraus[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg, Germany — [2]ZAE Bayern, D-97074 Würzburg, Germany

The highest efficiencies reported for organic solar cells are for devices incorporating blends of conjugated polymers and C_{70}-derivatives, due to their higher optical absorption compared to C_{60}. Yet the costly purification of higher fullerenes might hinder a widespread adoption of this promising material. However recent results showed that polymers blended with a PC$_{60}$BM/PC$_{70}$BM mixture without further purification yield solar cells with comparable performance. This is surprising, because from absorption and photoluminescence spectra, different energy levels for both fullerenes are expected. If there were a noticeable difference in electron affinity, one of the two fullerenes would act as an electron trap in a mixed phase, hence hindering transport and limiting device performance. This raises the question, on which fullerene derivate the electron is residing after light induced charge transfer from the polymer? Using Light-induced Electron Spin Resonance (LESR) we can distinguish between holes on the polymer and electrons on either C_{60} or C_{70}, since their ESR spectra are slightly shifted against each other. Our results demonstrate that there is no strong preference for either fullerene. Thus from an economic point of view “unpurified” fullerenes might be a viable option for large scale production.

CPP 18.5 Wed 10:30 C 130

Exciton and Charge Dynamics in PCPDTBT:PCBM Blends Probed by Broadband VIS-NIR Transient Absorption Spectroscopy — •Fabian Etzold, Ian A. Howard, Don Cho, Michael Meister, Ralf Mauer, Klaus Müllen, and Frédéric Laquai — MPI für Polymerforschung Mainz

The efficiency of PCPDTBT:PCBM bulk heterojunction solar cells depends very much on the film preparation conditions, like the use of cosolvents, for reasons still not well understood. In this contribution we present the exciton and charge carrier dynamics in pristine PCPDTBT films and in photovoltaic blends with PCBM studied by VIS-NIR broadband transient absorption spectroscopy. In particular we monitor the previously unobserved, but for low-bandgap polymers essential spectral region between 1000-2000 nm, where we can clearly identify the individual contributions and dynamics of singlet excitons, charge-transfer excitons as well as free and trapped polarons. This not only allows a qualitative assessment of the effect of cosolvents on the photophysics, but also the extraction of the most relevant recombination parameters that finally determine the device efficiency. Our experiments show that cosolvents promote the generation of mobile charge carriers that can be extracted as photocurrent.

[1] F. Etzold et al., manuscript in preparation.

CPP 18.6 Wed 10:45 C 130

Origin of Sub-Bandgap Absorption in P3HT:PCBM Solar Cells — Martin Presselt, •Felix Herrmann, Marco Seeland, Maik Bärenklau, Roland Rösch, Wichard J. D. Beenken, Erich Runge, Sviatoslav Shokhovets, Harald Hoppe, and Gerhard Gobsch — TU Ilmenau, Ilmenau, Germany

To explain the origin of sub-bandgap (SBG) absorption contributing to the photocurrent in bulk-heterojunctions (BHJ) made of poly(3-hexylthiophene-2,5-diyl) (P3HT) and [6,6]-phenylC61-butyric acid methyl ester (PCBM) at least four different models are discussed in the literature. In an earlier work we have shown that an exponential in addition to a Gaussian function is needed to reproduce SBG external quantum efficiency (EQE) spectra. There, the exponential function was assigned to a disorder related absorption tail, while the SBG EQE Gaussian was not assigned unambiguously. In the present work, the SBG EQE Gaussian is assigned to a hole-polaron transition at P3HT rather than to a direct charge transfer transition from the P3HT HOMO to the PCBM LUMO or absorption of molecularly dispersed PCBM as concluded from temperature dependent EQE measurements.

CPP 19: Charged Soft Matter

Time: Wednesday 9:30–11:00 Location: C 243

CPP 19.1 Wed 9:30 C 243

Structure and Dynamics of Polyelectrolytes in Aggregates with oppositely charged Surfactants — •Ingo Hoffmann[1,2], Bela Farago[2], Norman J. Wagner[3], and Michael Gradzielski[1] — [1]TU Berlin, Berlin, Germany — [2]Institut Laue Langevin, Grenoble, France — [3]University of Delaware, Newark, USA

Systems composed of oppositely charged polyelectrolytes and surfactants show rich self-aggregation behavior that varies over a large size range and have many applications e.g. in cosmetics, detergency and drug delivery. Mixtures of the cationic polyelectrolyte JR 400 with anionic surfactants (SDS, SDBS) in the semi-dilute regime with a slight excess of polymer charges form highly viscous network structures. In this study we investigated the structure and dynamics of the aggregates and its individual components i.e., the polyelectrolyte chain and the surfactant, with the aid of small-angle neutron scattering (SANS) and neutron spin-echo (NSE). Neutron scattering provides the unique ability to match the contrast of a certain component with that of the solvent by changing its isotopic composition and thereby rendering it *invisible*. This is achieved bu using a deuterated surfactant (d-SDS) and an appropriate mixture of H_2O and D_2O as solvent.

In summary, we studied the behaviour of polyelectrolytes in solutions of mixed aggregates of polyelectrolytes and oppositely charged surfactants using neutron scattering to gain an understanding of the role of the individual components in the formation and dynamics of such aggregates. This understanding can be valuable for the design of future formulations.

CPP 19.2 Wed 9:45 C 243

Weak polyelectrolyte adsorption onto oppositely charged interfaces: planar, cylindrical, and spherical geometries. — •Andrey Cherstvy and Roland Winkler — Institute of Complex Systems, ICS-2/IAS-2, Forschungszentrum Jülich, 52425 Jülich, Germany

We suggest a universal description for weak adsorption of flexible polyelectrolytes (PE) onto oppositely charged planar and curved surfaces [Phys. Chem. Chem. Phys., 13 11686 (2011)]. The analysis is based on the WKB quantum mechanical method for the Green function equation. We provide a unified picture for scaling behavior of the critical characteristics and thickness of adsorbed PE layer formed near the interfaces. We find that curved convex interfaces necessitate much higher surface charge densities to trigger the PE adsorption. Different geometries also yield distinct scaling laws for the critical surface charge density $\sigma^\star$. Namely, at low-salt $\sigma^\star$ scales cubical with the inverse Debye screening length for a plane, quadratic for an adsorbing rod, and linearly for a sphere. These novel scaling trends for PE-rod and PE-sphere adsorption are consistent with the complex formation experiments from P. Dubin lab. Above the adsorption threshold, the thickness of the adsorbed PE layer predicted is consistent with other theoretical models. Our analysis can provide a more realistic description of adsorption of charged biopolymers at biologically-relevant conditions.

CPP 19.3 Wed 10:00 C 243

Simulations of charged dendrimer-linear polyelectrolyte complexes with explicit counterions — •Jarosław Sylwester Kłos[1,3] and Jens Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany — [2]Institute for Theoretical Physics, Technische Universität Dresden, 01069 Dresden, Germany — [3]Faculty of Physics, A. Mickiewicz University, Umultowska 85, 61-614 Poznan, Poland

We study complexes comprised of one $G4$ dendrimer with $N_t = 32$ positively charged end groups and an oppositely charged linear polyelectrolyte accompanied by 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 with the reduced temperature τ and chain length N_{ch} as the simulation parameters. Our calculations indicate three temperature ranges that determine the behavior of such complexes. At $\tau_{complex}$ complexes are formed first, which are accompanied by selective counterion localization within the complex at $\tau_{loc} \leq \tau_{complex}$. Counterion condensation takes place as temperature is decreased below $\tau_{cond} < \tau_{loc}$. We observe that condensation occurs exclusively on the excess charges in the complex and thus no condensation is observed at the compensation point ($N_{ch} = N_t$) no matter τ. For $N_{ch} \neq N_t$ the complex is overally charged. We also find that more rigid chains take a variety of shapes including oblate, spherical and rodlike ones. At low τ a sharp release of tails by long chains is detected by increasing their rigidity.

CPP 19.4 Wed 10:15 C 243

Electro-kinetics of Charged Sphere Suspensions Explored by Integral Low Angle Super-Heterodyne Laser Doppler Velocimetry — •Bastian Sieber, Holger Schweinfurth, Tetyana Köller, and Thomas Palberg — Johannes Gutenberg Universität, D-55128 Mainz, Germany

We investigated the flow behaviour of colloidal charged-sphere suspensions using a newly designed integral low angle super-heterodyne laser Doppler velocimetry which combines the advantages of several previous approaches. The obtained power spectra correspond to diffusion broadened velocity distributions across the complete sample cross section. The excellent performance of the instrument is highlighted in detail at the example of electro-kinetic flow of suspensions in a closed cell of rectangular cross section. We demonstrate that our instrument allows for convenient and simultaneous quantitative determination of the electro-phoretic mobility, the electro-osmotic mobility, the particle flow profile, an effective diffusion coefficient, and the spectral power as a function of interaction conditions.

CPP 19.5 Wed 10:30 C 243

Diffusion of nanoparticles at an air/water interface is not invariant under a reversal of the particle charge — •Tobias Gehring and Thomas M. Fischer — The University of Bayreuth, Germany

The diffusion of charged nanoparticles at an aqueous/air interface is not invariant under a charge reversal of the particles. Negatively charged particles slow down with the ionic strength of the aqueous phase, while positively charged particles speed up. The diffusion constant of the particles reflects their immersion into the aqueous/air interface. We argue that the opposing behavior of oppositely charged particles is proof that the immersion depth of the particles scales with the contrast in electric surface potential of the particle to the electric surface potential of the air/water interface, not with the particle*s charge density. We therefore propose to incorporate the potential drop across the air/water interface into theories of electrodipping.

CPP 19.6 Wed 10:45 C 243

Enhanced charge transport in nano-confined ionic liquids — •Ciprian Ghiorghita Iacob, Joshua Sangoro, Wycliffe Kipnusu, Rustem Valiullin, Jörg Kärger, and Friedrich Kremer — Institute of Experimental Physics I, University of Leipzig, Leipzig, Germany

Charge transport in ionic liquids contained in unidirectional nanoporous membranes (pore diameters: 7.5-10.4 nm) is investigated by combining Broadband Dielectric Spectroscopy (BDS) and Pulsed Field Gradient (PFG)-NMR [1-3]. This enables one to determine the diffusion coefficient and the diffusion rate over more than 13 decades and to trace its temperature dependence [4, 5]. Under conditions of nanometric confinement, a change from a Vogel-Fulcher-Tammann into an Arrhenius-like thermal activation is observed, resulting in an enhancement of diffusivities by more than two orders of magnitude. The effect becomes more pronounced with decreasing pore diameter. It is attributed to changes in molecular packing and hence in density leading to higher mobility and electrical conductivity.

References 1. Iacob, C.et al., Phys. Chem. Chem. Phys.,12(41): p. 13798-13803,2010. 2. Iacob, C.et al., Soft Matter, 2011. 3. Kremer, F., Schönhals, A.,Berlin: Springer,2003. 4. Sangoro, J.R. and Kremer, F.,Accounts of Chemical Research, 2011. 5. Sangoro, J.R., et al. Soft Matter, 7(5): p. 1678-1681, 2011.

CPP 20: (Hydro)gels and Elastomers

Time: Wednesday 9:30–11:00 Location: C 264

CPP 20.1 Wed 9:30 C 264

Kinetics of structural changes in thermoresponsive block-copolymer solutions — Joseph Adelsberger[1], Ezz Metwalli[1], Alexander Diethert[1], Achille M. Bivigou-Koumba[2], André Laschewsky[2], Isabelle Grillo[3], Peter Müller-Buschbaum[1], and •Christine M. Papadakis[1] — [1]TU München, Physikdepartment, Physik weicher Materie, Garching — [2]Universität Potsdam, Institut für Chemie — [3]Institut Laue-Langevin, Grenoble

Thermoresponsive polymers exhibit lower critical solution temperature (LCST) behavior and are of great interest for applications in ultrafiltration, in sensors or in transport/delivery systems.

We have studied triblock copolymers consisting of two hydrophobic polystyrene end blocks and a hydrophilic poly(N-isopropyl acrylamide) middle block. In aqueous solution, they form core-shell micelles or micellar networks [1]. The structural changes occurring after rapid heating above the cloud point were followed using time-resolved small-angle neutron scattering experiments [2]. Both, the polymer concentration and the target temperature were varied. The PNIPAM shell shrinks and releases water very rapidly. The collapsed micelles form small fractal aggregates, which become denser. Their growth first follows the diffusion-limited aggregation, whereas later, the clusters grow by coagulation. Depending on the target temperature, a skin effect is observed at the cluster surface.

[1] J. Adelsberger, C. M. Papadakis et al., Macromolecules 43, 2490 (2010). [2] J. Adelsberger, C.M. Papadakis et al., Macromol. Rapid Commun., accepted.

CPP 20.2 Wed 9:45 C 264

Phase transition behaviour of different aqueous poly(N-isopropylacrylamide) systems monitored by dielectric spectroscopy — •Marieke Füllbrandt[1], Regine von Klitzing[2], and Andreas Schönhals[1] — [1]BAM Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12205 Berlin — [2]Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Strasse des 17. Juni 124, 10623 Berlin

Dielectric Relaxation Spectroscopy (DRS) is applied in a broad frequency range at temperatures between 15°C to 50°C to aqueous solutions of linear Poly(N-isopropylacrylamide)(pNIPAM) with different polymer concentrations and to aqueous dispersions of pNIPAM microgels with different crosslinking densities. In aqueous media thermosensitive pNIPAM shows a lower critical solution temperature (LCST) at about 32°C where it changes its properties from hydrophilic to hydrophobic. The phase transition of pNIPAM can be monitored by both the temperature dependence of the DC conductivity and the frequency dependence of the conductivity spectra. The latter one is due to a Maxwell/Wagner/Sillars polarization and can be related to the change in chain or particle structure at the LCST of pNIPAM. The frequency and temperature dependence of the conductivity was investigated in dependence on the polymer concentration for linear pNIPAM and on the crosslinking density for pNIPAM microgels. The dielectric measurements were accompanied by dynamic light scattering (DLS) and zeta potential measurements in order to relate the dielectric data with results obtained by well established methods.

CPP 20.3 Wed 10:00 C 264

A comparison of the morphology and thermoresponsive switching behavior in thin films of cyclic and linear poly(N-isopropylacrylamide) — •David Magerl[1], Xing-Ping Qiu[2], Françoise M. Winnik[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik -Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]Université de Montréal, Faculty of Pharmacy and Department of Chemistry, CP 6128 Succursale Centre Ville Montréal QC H3C 3J7, Canada

Stimuli-responsive hydrogels are of increasing interest because of their use in a variety of applications such as switches and sensors. Poly(N-isopropylacrylamide) (PNIPAM) is one of the most studied polymers in this context. However, there are only very few studies on cyclic PNIPAM, although this topology is of great interest because of the absence of end-groups, which has a significant impact on the lower critical solution temperature (LCST).

In this study, we compare the properties of spin-coated thin films of cyclic and linear PNIPAM samples with similar molecular weights and a low polydispersity. The film thickness is varied and the films are characterized with x-ray reflectivity and optical microscopy. The swelling behavior of these films, exposed to water vapor, is investigated as a function of film thickness in order to assess the influence of chain topography on the thin film behavior. Additionally, the interface correlation between the surface and the substrate is probed with grazing incidence small-angle x-ray scattering.

CPP 20.4 Wed 10:15 C 264

Determination of viscoelastic properties of adsorbed thermo responsive gel particles via AFM tip indentation — •Marcel Richter and Regine von Klitzing — TU Berlin, Straße des 17.Juni 124, 10623 Berlin

During the last decades microgels made of N-isopropylacrylamide (NIPAM) have attracted much interest and were studied by several techniques like atomic force microscopy (AFM) and dynamic light scattering (DLS) [1]. These polymer particles show thermo responsive behaviour and can therefore be classified as "smart" materials. For the later adsorption behaviour of nano- and micro-objects like colloidal particles or cells on top of adsorbed microgel layers the mechanical properties of such microgels are of great interest. Here, the AFM tip indentation method is a suitable method for the determination of the Young's modulus [2]. We synthesised microgel particles with different co-monomers and study the stiffness according to the cross linker and co-monomer amount. The measurements show a tremendous shift in the lower critical solution temperature (LCST) and change in (visco) elasticity. The size of microgels is determined by Dynamic Light Scattering and Scanning Force Microscopy.

[1] K. Kratz, T. Hellweg, W. Eimer, Polymer (2001), 42, 6531

[2] E. K. Dimitriadis et al, Biophysical Journal, (2002), 82, 2798

CPP 20.5 Wed 10:30 C 264

Computersimulations of Magnetic Gels — •Rudolf Weeber[1], Sofia Kantorovich[1,2], and Christian Holm[1] — [1]Institute for Computational Physics, University of Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart, Germany — [2]Ural Federal University, Lenin Avenue 51, 620000 Ekaterinburg, Russia

Magnetic gels consist of magnetic nano-particles embedded in a cross-linked polymer network. They have potential applications ranging from medicine to engineering, such as drug release systems and artificial muscles. These applications rely on the combination of the mechanical properties of the polymer network with the ability to modify and control the sample with external magnetic fields due to the embedded magnetic nano-particles.

Today, many aspects of the synthesis of ferrogels are understood and the properties of gels can be characterized and tailored. However, many questions concerning the microstructure and its influence on macroscopic properties of magnetic gels are still open. Here computer simulations can help since they allow to study simplified model systems which focus on certain characteristic features of the material.

In this contribution we present computer models which demonstrate different mechanisms of deformation and changing elastic properties of a ferrogel in an external magnetic field. They help to explain the contradicting findings for the shape change of magnetic gels observed in experiments.

CPP 20.6 Wed 10:45 C 264

Polymer Dynamics and Crosslink Density of SBR Nanocomposites Containing Fillers with Different Surface Area — •Anas Mujtaba[1], Melanie Keller[2], Sybill Ilisch[2], Hans-Joachim Radusch[2], Thomas Thurn-Albrecht[1], Kay Saalwächter[1], and Mario Beiner[1] — [1]Faculty of Natural Sciences II, Martin-Luther-University Halle-Wittenberg, Germany — [2]Center of Engineering Sciences, Martin-Luther-University Halle-Wittenberg, Germany

Styrene butadiene rubber (SBR) samples filled with different amounts of silica nanoparticles or mixtures of high-surface silica and low-surface borosilicate particles are investigated by dynamic shear measurements and solid state NMR. Aim is to study the influence of filler surface area on the properties of the SBR composites. Double-quantum NMR data are used to determine crosslink densities. Absolute values for the crosslink densities of SBR composites are calculated using additional information from shear measurements on unfilled samples. The effective crosslink density of the SBR matrix is slightly decreasing if filler content or filler surface area increases. Shear data show that substituting high- with low-surface area silica at constant volume fraction is not only affecting reinforcement and plateau modulus but also energy dissipation in the plateau range. Glass temperature and frequency temperature position of the main transition α of SBR composite, however, are not much affected. Dynamic strain sweeps in the plateau reveal the contribution of the filler network which breaks at large deformations.

CPP 21: Poster: Wetting, Micro and nanofluidics

Time: Wednesday 11:00–13:00 Location: Poster A

CPP 21.1 Wed 11:00 Poster A

Forced Displacement Experiments in quasi 2D Porous Media — •Michael Jung[1,2], Marta Sanchez de la Lama[2], Stephan Herminghaus[2], Martin Brinkmann[2], and Ralf Seemann[1,2] — [1]Universität des Saarlandes, Saarbrücken, Germany — [2]Max Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany

As a simple model for a forced liquid displacement process into porous media, we study two-dimensional flow experiments in microfluidic devices. The devices and the porous structure are fabricated from oil-resistant UV-curable glue using a soft-lithography technique. These devices were first saturated with oil of different viscosities and densities (silicon oils or alkanes). The oil was then displaced by flushing water of ether different flow rates or at an adjustable constant pressure. To precisely distinguish between the oily and the aqueous phase we add a dye to the aqueous phase. We observe the global and local dynamic behavior of liquid front using high speed microscopy. The effect of various additional parameters, such as wettability and the size and geometry of the pore space on the position and the roughening of the liquid front as well as the remaining fraction of trapped oil was investigated in detail. Parallel to the experiments we are studying numerically the effect of porosity and wetting conditions on two dimensional two phase flows in porous media. To this end we employ a multiple particle collision method for immiscible liquids that allows to vary the wettability of the pore walls.

CPP 21.2 Wed 11:00 Poster A

Liquid Morphologies in granulates with various wettability — •Marc Schaber[1], Mario Scheel[3], Martin Brinkmann[2], Marco Di Michiel[3], and Ralf Seemann[1,2] — [1]Experimental Physics, Saarland University, D-66041 Saarbrücken — [2]MPI for Dynamics and Self-Organization, D-37073 Göttingen — [3]European Synchrotron Radiation Facility, F-38000 Grenoble

When adding liquid to dry granulates, the liquid forms a network of capillary bridges and complex liquid structures. Depending on wettability of the granules and geometry of the granular pile different liquid structures are formed. By means of X-ray micro-tomography we explore the liquid equilibrium distribution emerging within granular packs. Monodisperse and polydisperse glass and basalt microspheres are used as granules having small and large contact angle, respectively. By fluidizing the granulate the packing geometry of the granules is changed and the liquid equilibrium structures are destroyed. Using ultra-fast X-ray tomography we explore how the liquid is re-distributed and how the liquid morphologies are re-formed in a new equilibrium situation.

CPP 21.3 Wed 11:00 Poster A

Wetting of grooved elastic substrates — •Carsten Herrmann[1], Dominik Michler[2], Martin Brinkmann[2], and Ralf Seemann[1,2] — [1]Experimental Physics, Saarland University, D-66041 Saarbrücken — [2]MPI for Dynamics and Self-Organization, D-37073 Göttingen

Wetting morphologies on grooved elastic substrates are considered experimentally. 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 of the emerging wetting morphologies caused by the virtue of capillary forces and the shape of the liquid morphologies as function of wettability and geometry. 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 particular lateral ordering of the wetting morphologies. We try to understand the mechanism causing the lateral ordering which are either a result of an energetic minimum or due to a frustration process.

CPP 21.4 Wed 11:00 Poster A

Microparticle Separation in Droplet Based Microfluidics — •Michael Hein[1], Jean-Baptiste Fleury[1], and Ralf Seemann[1,2] — [1]Experimental Physics, Saarland University, D-66041 Saarbrücken — [2]MPI for Dynamics and Self-Organization, D-37073 Göttingen

To compartment extremely small liquid volumes into droplets and manipulate them in droplet based microfluidic systems offers the benefit of inhibiting dispersion and cross contamination of analytes. For many applications like cytometry, hemotology or immunoassays molecules are attached to microbeads and subsequently dispersed in various liquids to achieve and probe certain reactions. To include those type of reactions into microfluidics devices we explore particle separation in droplets flowing in straight microfluidic channels. Particle separation might occur inside a droplet and leads to a concentration of dispersed particles at either the front or the rear end of a droplet after a short travel distance. We explore the particle separation for several parameters like density difference of the particles and the dispersed phase, particle size, viscosities of the liquids, droplet size, channel geometry, and flow velocity. After concentrating the particles, the droplet can be split into fractions containing excess dispersed phase and a large concentration of particles, which then can be used for further microfluidic processing or analyses.

CPP 21.5 Wed 11:00 Poster A

Microfluidic Platform for Membrane Fusion Studies — •J. Nabor Vargas[1], Jean-Baptiste Fleury[1], and Ralf Seemann[1,2] — [1]Experimental Physics, Saarland University, D-66041 Saarbrücken — [2]MPI for Dynamics and Self-Organization, D-37073 Göttingen

Membrane fusion is essential for the life of eukaryotic cells, it is known as the process whereby two separate lipid bilayers merge to become one by means of a family of fusogenic proteins. Research on membrane fusion has been intense along past decades, but we are still far from unveiling the whole phenomena. We are exploring a new microfluidic approach to study single membrane fusion events in a controllable geometry. This experimental setup shall allow for the production of stable lipid bilayers, easy variation of the lipid membrane composition like the insertion of proteins, and superior control of the fusion process by e.g. by optical and electrical access. Lipid bilayers created inside the microfluidic chip can be moved and manipulated making them interact with each other resembling cell membrane fusion.

CPP 21.6 Wed 11:00 Poster A

Simulation of droplet traffic in asymmetric microfluidic loop — •Erfan Kadivar, Stephan Herminghaus, and Martin Brinkmann — Max Planck Institute for Dynamics and Self-Organization, Fassberg 17, D-37077, Göttingen, Germany

As observed in the recent experiments, the repartition of droplets at the inlet of an asymmetric microfluidic loop depends on the droplet size and distance of consecutive droplets [1-2]. In this work we present a numerical study of the droplet traffic at microfluidic channel with an asymmetric loop. As we assume the flat channel, we consider the flow in the Hele-Shaw limit, where the dynamics of two phases can be described by an effectively two dimensional Darcy flow. The continuity equation in combination with Darcy's law provides a self-consistent integral representation of the pressure on the boundary of the droplets and the side walls of the channels which is solved using standard boundary element methods. In addition to the Laplace pressure, we consider a disjoining pressure acting on the interface touching the interface of another droplet or the side wall. Finally we calculate the fraction of droplets flowing through in each arm of the loop as function of droplet size, arm length ratio, and distance between two consecutive droplets.

[1] M. Belloul, and et al, Soft Matter 7, 9453 (2011).

[2] W. Choi, and et al, Lip on a Chip 11, 3970 (2011).

CPP 21.7 Wed 11:00 Poster A

Microfluidic investigation of the electric-field-induced Frederiks transition in nematic liquid crystals in conjunction with a flow field — •Pramoda Kumar, Anupam Sengupta, and Christian Bahr — Max-Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany

Microfluidic studies of nematic liquid crystals (LCs) offer interesting insights into hydrodynamics of anisotropic fluids, dynamics of topological defects and effects of confinement and surface anchoring of LC molecules on experimental outcomes [1,2,3]. In the present study, we use microfluidics to investigate the effect of flow on the electric-field-induced Frederiks transition in nematic liquid crystals. Depending on the direction of the applied electric field with respect to the equilibrium orientation of the LC molecules in flow, the orientational effects of the electric field can be either enhanced or reduced by varying the flow velocity. Effectively, we demonstrate the competing effects between flow and electric field induced orientation of the LC molecules. By tuning the flow velocity, the threshold voltage of the Frederiks transition can be adjusted. This phenomenon can be potentially utilized in display industry where there is an ever growing need for low energy consumption coupled with low response times.

[1] C. J. Holmes, S. L. Cornford and J. R. Sambles, Phys. Rev. Lett. **104**, 248301 (2010).

[2] A. Sengupta, S. Herminghaus and Ch. Bahr, Mol. Cryst. Liq. Cryst. **547**, 203 (2011).

[3] A. Sengupta, U. Tkalec and Ch. Bahr, Soft Matter **7** 6542 (2011).

CPP 21.8 Wed 11:00 Poster A

Dynamics of liquid-liquid dewetting — •Stefan Bommer[1], Sebastian Jachalski[2], Dirk Peschka[2], Barbara Wagner[2], and Ralf Seemann[1] — [1]Saarland University,Saarbrücken — [2]Weierstrass Institute, Berlin

We investigate the dewetting behavior of liquid polystyrene films (PS) from an underlying liquid poly(methyl)acrylate (PMMA) substrate. To understand the dynamics and the characteristics of liquid-liquid dewetting we explore the entire dewetting process from film rupture to the final droplet shape by in-situ scanning force microscopy (AFM). The nanometric polymer films are prepared in an non-equilibrium, glassy state and the dewetting process is started by heating the polymer films above their respective glass transition temperatures. The system is solidified by a fast reduction of temperature and the solidified liquid-liquid interface can be imaged by AFM after removing the upper PS structures using a selective solvent. Correlating both interfaces the 3d-shape of the dewetting structures can be determined. From the equilibrium droplet shapes and the resulting contact angles we can e.g. determine the ratio of the interfacial energies. The thus determined parameters are used as input parameter for numerically simulated dewetting processes which are compared to experimental results.

CPP 21.9 Wed 11:00 Poster A

Forced wetting of simple and complex fluids in horizontal capillaries — •Manos Anyfantakis[1], Günter K. Auernhammer[1], Daniela Fell[1,2], Mohammad A. Dadfar[1], and Hans-Jürgen Butt[1,2] — [1]Max Planck Institute for Polymer Research — [2]Center of Smart Interfaces, Technical University of Darmstadt

Investigation of the physics governing the dynamic wetting of various liquids in cylindrical capillaries is of profound interest in numerous practical applications, such as microfluidic devices, oil extraction, and printing technologies as well as various medical applications. Additionally to spontaneous wetting of microchannels, forced capillary wetting could provide a straightforward way to systematically address questions in dynamic wetting of simple and complex fluids. Here, we describe a simple method, which allows for the simultaneous measurement of both the advancing and the receding contact angles of moving liquid slugs.

The experimental setup consists of three main parts: the liquid reservoir, the glass capillary and a microscope equipped with a fast camera, which is used to image the moving liquid slugs. The driving force for liquid motion is the gravity induced pressure difference between the reservoir and the microscope stage. The advancing/receding contact angles are determined either by placing the local tangent to the triple line-liquid-gas interface or by fitting the meniscus shape. Experimental results regarding dynamic wetting/dewetting of surfactant solutions in capillaries of different wettabilities, in a broad speed range, are as well as challenges and further possibilities of the method are discussed.

CPP 21.10 Wed 11:00 Poster A

Gas flow measurements in nanopores: The influence of pore wall roughness on gas dynamics — •Sebastian Kiepsch[1], Simon Gruener[1,3], and Patrick Huber[1,2] — [1]Universität des Saarlandes, Experimentalphysik, Saarbrücken, Germany — [2]Pontificia Universidad Católica de Chile, Facultad de Física, Santiago, Chile — [3]BASF SE, Ludwigshafen, Germany

We have measured the flow of rarefied helium gas through various nanoporous membranes within a broad temperature range ($30-300\,\mathrm{K}$). The materials used for these experiments (anodized aluminium oxide and Vycor glass) featured typical pore diameters in the range from $13-50\,\mathrm{nm}$. The results were found to be in accordance with numerical calculations, based on a Knudsen diffusion model for cylindrical cross-sections. For Vycor glass, a tortuosity factor of $\tau = 3.6 \pm 0.05$ of the pore-network could be measured. In order to determine the influence of wall roughness on gas dynamics, the samples were reversibly modified by means of low-temperature argon vapour condensation. In this way we were able to add a monolayer of argon to the pore walls. Subsequent flow measurements with helium gave hints of higher diffusion coefficients. This effect may be related to pore wall smoothing upon argon adsorption.

CPP 21.11 Wed 11:00 Poster A

Pore Scale Investigations Of Forced-Imbibition In Porous Media — •Hagen Scholl[1], Kamaljit Singh[2,3], Marco Di Michiel[3], Mario Scheel[3], Stephan Herminghaus[2], and Ralf Seemann[1,2] — [1]Saarland University, Experimental Physics, D-66041 Saarbrücken, Germany — [2]MPI for Dynamics and Self-Organization, D-37073 Göttingen, Germany — [3]ESRF, BP 220, F-38043 Grenoble, France

We investigate static and quasi-static liquid morphologies of immiscible-liquid (water-oil) fronts in an initially oil saturated bead matrix flooded by water using ultra-fast X-ray micro-tomography at the European Synchrotron Radiation Facility (ESRF, ID15). The data were analysed for change in residual oil morphologies, the shape of liquid front with time during continuous water flooding and various factors affecting its behaviour, such as wettability (glass/basalt beads), flow rates, pore geometry and the influence of gravity. Our results show that the water-oil front is more compact in basalt beads, whereas the front in glass beads progresses in elongated fingers. The fingering in the porous medium results in a higher final residual oil saturation for glass beads, after a complete water flood due to bypassing of several oil-filled pore pockets. Preliminary results indicate a crucial importance of the wettability and that the front behaviour seems to be dominated by capillary forces, whereas the flow rate doesn't play a major role.

CPP 21.12 Wed 11:00 Poster A

Nanoscale pumping of water by AC electric fields — •Klaus Rinne[1], Stephan Gekle[2], Douwe Jan Bonthuis[2], and Roland Netz[1] — [1]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — [2]Technische Universität München, 85748 Garching, Germany

Using molecular dynamics simulations we present a novel mechanism for pumping of water through a carbon nanotube by time-dependent electric fields. The fields are generated by electrodes with oscillating charges in a broad GHz frequency range which are attached laterally to the tube. The key ingredient is a phase shift between the electrodes to break the spatio-temporal symmetry. A microscopic theory based on a polarization-dragging mechanism accounts quantitatively for our numerical findings.

CPP 21.13 Wed 11:00 Poster A

Measuring Flow Properties in Porous Media With Micron-sized Colloidal Tracers — •Christian Scholz[1], Frank Wirner[1,2], and Clemens Bechinger[1,2] — [1]2.Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Max-Planck-Institut für Intelligente Systeme, Heisenbergstraße 3, 70569 Stuttgart, Germany

The understanding of transport and flow phenomena in porous media is important for many problems which arise in various fields of science and engineering, ranging from agricultural, biomedical, chemical and petroleum engineering to soil sciences. Although the literature on porous media has been growing rapidly over the last decades it is still unclear, how transport properties of liquids through porous materials can be related to their structure. We use finite-sized colloidal tracers to study flow and transport properties in random quasi-2D microfluidic porous media and study the effects of the tracer size on the mean and local tracer velocity within such structures. Significant differences in the mean velocities of different-sized tracers are found even for very low Stokes numbers, due to differing particle height distributions. We discuss the implications of these deviations for permeability measurements from particle tracking velocimetry. By applying an exponentially decreasing pressure drop we overcome the size dependence and measure the permeability of porous structures independently of tracer-size effects in the structure.

CPP 21.14 Wed 11:00 Poster A

Flow induced surface attachment of gold nanorods as probed with microfluidics and in-situ GISAXS — •Volker Körstgens[1], Kuhu Sarkar[1], Gerd Herzog[2], Matthias Schwartzkopf[2], Adeline Buffet[2], Frans J. de Jong[3], Stephan V. Roth[2], Michael Schlüter[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]HASYLAB at DESY, 22603 Hamburg, Germany — [3]TU Hamburg-Harburg, IMS, 21073, Hamburg, Germany

The attachment of nanoparticles to a surface can be followed in-situ with GISAXS (grazing incidence small angle x-ray scattering) with a special designed microfluidic flow cell [1]. In this study the attachment of different gold nanoparticles including high aspect ratio gold nanorods to surfaces of insoluble calcium-alginate films is investigated. A scan along the microfluidic channel is carried out, collecting scattering data at different positions. With the brillant x-ray source available at the beamline MiNaXS of the PETRA III synchrotron source this procedure offers a time resolved as well as a position resolved GISAXS investigation of the attachment of nanoparticles. Information about the flow induced orientation of the attached high aspect ratio nanoparticles can be deduced from the GISAXS experiments.

This work has been financially supported by the BMBF (grant number 05K10WOA).

[1] J.-F. Moulin et al., Rev. Sci. Instrum. 79, 015109 (2008).

CPP 21.15 Wed 11:00 Poster A

Electrowetting on 3-dimensional structures: A method to control the transport of liquid plugs through hydrophobic sieves — •Markus Wink[1,2], Thomas Palberg[1], Karin Potje-Kamloth[2], and Michael Bassler[2] — [1]Johannes Gutenberg University Mainz, Germany — [2]Institut für Mikrotechnik Mainz, Germany

In the last two decades electrowetting has made its way into new applications, e. g., "lab-on-a-chip" systems, display technologies and microlenses. Recently, Lifton et al. have shown the use of electrowetting in microbatteries by introducing a micropourous structure, which is actively switched to the wetting state [1]. Here, we apply electrowetting to a microfluidic system and show tunable wetting and subsequent dewetting of a sieve representing a fundamental 3-dimensional structure. The pressure curve for transport of a liquid plug through a sieve is analytically described for a square mesh. The liquid entry pressure (LEP), which is the pressure required to fully wet the pores, depends on the size and shape of the pores, the interfacial tension of the liquid and the contact angle of the liquid on the solid surface. To enable electrowetting the square mesh is coated with a dielectric layer for electrical isolation and the surface is functionalized with a hydrophobic layer. The apparent contact angle of droplets on the sieve is investigated as a function of voltage. In addition, the LEP as a function of voltage is determined to test our hypothesis of a reduced LEP under electrowetting conditions.

[1] V.A. Lifton et al., Appl. Phys. Lett. 93, Issue 4 (2008) 043112

CPP 21.16 Wed 11:00 Poster A

Three-dimensional imaging of water drops on hydrophobic surfaces by confocal microscopy — •Periklis Papadopoulos, Hans-Jürgen Butt, and Doris Vollmer — Max Planck Institut for Polymer Research, Mainz, Germany

The microscopic description of wetting of a rough or structured solid surface by a liquid is still a challenge. Nano- and micrometer-sized inhomogeneities cause pinning of the three-phase contact line, preventing drops to reach their global equilibrium. To investigate the relation between the local, microscopic and the macroscopic contact angle, we image water drops on microstructured surfaces by laser scanning confocal microscopy (LSCM). The microstructures consist of cylindrical pillars arranged in a square lattice. Both the substrate and water are fluorescently labeled, allowing for accurate imaging of all interfaces and the three-phase contact line. Contact angles can be measure with accuracy of 1° and spatial resolution of a few μm. The "microscopic" contact angle close to the substrate varies by up to 30° along the wetting line, depending on the precise position. This variation, along with the contact line profile, causes deviations of the drop shape that persist at heights more than one magnitude larger than the size of the microstructures. This detailed information will allow us to tune the wetting properties of rough and patterned surfaces.

CPP 21.17 Wed 11:00 Poster A

Microfluidic systems for surface tension measurement — •Quentin Brosseau and Jean-Christophe Baret — Max Planck Institut for Dynamics & Self-organization, Göttingen, Germany

With the increasing number of microfluidics droplet-based methods developed, understanding surfactant adsorption at droplet interfaces, as main stabilizing process of emulsions, has become a major concern. Although such processes are well described in the diffusional case, models does not apply on chip where convective circulation is present. Our project aims at developing a series of microfluidic tools providing insights into the dynamics of surfactant adsorption, down to the millisecond-scale, for a dynamic determination of droplets surface tension. We for example exert a localized hydrodynamic stress transversal to the flow direction on the droplet. The droplet response – in deformation and relaxation – is measured and studied. The measured droplet deformation profiles reveal the characteristic time for surfactant adsorption at the interface, and the adsorption-desorption equilibrium. The influence of surfactant concentration, both above and below the CMC, and of the liquid flow rate are measured and additional 2D numerical simulation of the droplet deformation profile, provide tools to link deformations to effective interfacial tension.

CPP 21.18 Wed 11:00 Poster A

Importance of Mechanical Properties in Two-Dimensional Flowing Crystals — •Jean-Baptiste Fleury[1], Ohle Caussen[2], Stephan Herminghaus[2], Martin Brinkmann[2], and Ralf Seemann[1,2] — [1]Experimental Physics, University of Saarland, Saarbrücken, Germany — [2]Max-Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

We study the mechanical response and the stability of monodisperse droplet packings in quasi 2d microchannels under longitudinal compression. Depending on the exact choice of parameter a considered static droplet arrangement can be mechanically unstable and segregates into domains of higher and lower packing fraction. This is of fundamental importance also for corresponding flowing systems as it is not possible to generate mechanically stable droplet trains in this fairly large region of accessible volume fraction (around 15%) [1]. As a consequence flowing droplet arrangements present complex non-equilibrium droplet rearrangements, in these parameter regions, arising from the coupling of interfacial instabilities and dissipative friction. We will experimentally and theoretically discuss these mechanisms of dynamical rearrangements in an out-of-equilibrium microfluidic system.

[1] J-B. Fleury, O. Caussen, S. Herminghaus, M. Brinkmann and R. Seemann, Appl. Phys. Lett. (to be published, 2011)

CPP 21.19 Wed 11:00 Poster A

Influence of surface modification on sputter deposition — •Berit Heidmann[1,2], Matthias Schwartzkopf[1], Mottakin M. Abul-Kashem[1], Gunthard Benecke[1,3], Adeline Buffet[1], Denise Erb[1], Gerd Herzog[1,2], Ezzeldin Metwalli[4], Jan Perlich[1], Andre Rothkirch[1], Kai Schlage[1], Peter Müller-Buschbaum[4], Ralf Röhlsberger[1], Wilfried Wurth[2], and Stephan V. Roth[1] — [1]Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, D-22607 Hamburg — [2]Univ. Hamburg, Inst. für Exp., Luruper Chaussee 149, 22761 Hamburg — [3]MPIKG, Dep. of Biomat., Am Mühlenberg 1, 14424 Potsdam-Golm — [4]TU München, Physik Department E13, James-Franck-Str. 1, 85748 Garching

Polymer-metal-nanocomposites are important for technical applications,e.g solar cells [1]. Metal sputter deposition on polymer templates represents one of the most efficient processes to obtain nanostructured composites. The crucial interaction is that of the metal atom with the polymeric material. We investigated in-situ the growth of gold cluster on top of these functionalized silanized silicon surfaces during sputter deposition under conditions similar to industrial processing. Using in-situ grazing incidence small-angle X-ray scattering, we show that due to different reaction mechanisms (chemisorption and physisorption) between the individual gold atom and the functional group yield different cluster growth kinetics, which in th case of thiol groups leads to the fast deposition of uniform gold layers.However, this is not the case in presence of phenyl groups due to their ability to repel gold atoms. [1] Kaune et al., ACS Apl. Mater. & Interfaces, 1, 353 (2009)

CPP 21.20 Wed 11:00 Poster A

Flow-stream-assisted deposition of gold nanoparticles — •Gerd Herzog[1,2], Mottakin M. Abul Kashem[1], Gunthard Benecke[1,3], Sebastian Bommel[1,4], Adeline Buffet[1], Frans J. de Jong[5], Volker Körstgens[6], Roman Mannweiler[1], Peter Müller-Buschbaum[6], Jan Perlich[1], Johannes F. H. Risch[1], Kuhu Sarkar[6], Matthias Schwartzkopf[1], Wilfried Wurth[2], and Stephan V. Roth[1] — [1]DESY, Notkestr. 85, D-22607 Hamburg — [2]Uni Hamburg, Inst. Exp.-P., Luruper Chaussee 149, D-22761 Hamburg — [3]MPI Coll. Int., Dep. Biomat., Am Mühlenberg 1, D-14476 Potsdam-Golm — [4]Humboldt-Uni Berlin, Institut für Physik, Newtonstr. 15, D-12489 Berlin — [5]TU Hamburg-Harburg, IMS, Eißendorfer Straße 38, 21073 Hamburg — [6]TU München, Physik-Dep. E13, James-Franck-Str. 1, 85747 Garching

Production of nanowires by deposition of gold nanoparticles via flow-stream technique onto a nanostructured polymer-coated substrate might offer a cheap and fast solution for industrial application [1]. We investigate the deposition of gold nanoparticles on colloidal polymeric samples with and without artificially induced μm-sized channels. Using a microfluidic cell in combination with in-situ GISAXS (beamline P03, Hamburg) we follow the gold deposition during the solution flow. First results indicate a different temporal nanoparticle layer growth compared to the three stages deposition on flat templates [2].

[1] Metwalli et al., Langmuir 2009, 25(19), 11815

[2] Roth et al., 1st Int. Symp. on Multiscale Multiphase Process Eng., Kanazawa (2011)(MMPE)

CPP 21.21 Wed 11:00 Poster A

Influence of solute–dependent wettability on the stability of films of mixtures and suspensions — •Desislava V. Todorova and Uwe Thiele — Department of Mathematical Sciences, Loughborough University, Loughborough, Leicestershire, LE11 3TU, UK

We discuss the behaviour of thin films of non-volatile liquid mixtures, colloidal suspensions and polymer solutions on a solid substrate. First, we reformulate the coupled long-wave time evolution equations for the film height and mean solute concentration for a 'passive' solute in gradient dynamics. This form can then be extended to incorporate additional effects [1]. In particular, we focus on a concentration-dependent wettability. It is determined employing homogenisation techniques to obtain effective optical characteristics [2]. Combining this with classical theory of effective molecular interactions between the film surface and the substrate, we arrive at a Derjaguin (or disjoining) pressure that depends on film height and concentration.

We use the derived model to study the linear stability of flat homogeneous films. In particular, we investigate how the stability thresholds are influenced by the incorporation of the additional degree of freedom related to the concentration field. As an outlook we also analyse nonlinear thickness and concentration profiles for steady droplets.

[1] U. Thiele, Eur. Phys. J. Special Topics 197, 213-220 (2011).

[2] G. A. Niklasson, C. G. Granqvist, O. Hunderi, Appl. Optics 20, 26-30 (1981); D. Todorova et al., J. Optoelectron. Adv. Mater. 11, 1296-1299 (2009).

We acknowledge support by the EU (PITN-GA-2008-214919).

CPP 21.22 Wed 11:00 Poster A

Influence of the wettability of the wall on capillary flow — Stefan Fogel, Ute Böhme, and •Ulrich Scheler — Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany

A Newtonian liquid in a capillary usually exhibits a parabolic flow profile resulting from the sticking at the wall. The situation is different in a capillary with a non-wetable wall. A significantly flattened profile is observed. Capillary flow is conveniently studied without any disturbance by flow NMR imaging. For each point in space velocity is determined in three directions. The focus has been on the transition between the two scenarios. Because a non-compressible liquid has been used, continuity requires transverse flow for the transition between the two flow profiles, which has been observed. Transition between the two types of flow profiles takes places over several millimeters and starts long before the change of the wall properties.

CPP 21.23 Wed 11:00 Poster A

Dynamic Contact Angles on Heterogeneous Substrates — •Daniel Herde, Stephan Herminghaus, and Martin Brinkmann — MPI for Dynamics and Self-Organisation, Goettingen, Germany

We study the influence of heterogeneities in the substrate wetting energy on the dynamical contact angle for a driven contact line. To this end, we model a 2-dimensional droplet sheared between two substrates in the Steady Stokes limit using boundary element methods.

Different definitions of the dynamic contact angle are compared. The constitutive velocity-contact angle relations for the case of driving with constant force and driving with constant velocity are discussed. Together with the information about the energy input in the system and the energy stored in the configuration of the free interface, we can characterise the influence of the heterogeneity on the energy dissipation in the system.

CPP 22: Poster: Charged Soft Matter

Time: Wednesday 11:00–13:00 Location: Poster A

CPP 22.1 Wed 11:00 Poster A

Liquid-liquid phase separation in protein solutions induced by YCl_3 — •Marcell Wolf[1], Fajun Zhang[1], Felix Roosen-Runge[1], Roland Roth[2], Maximilian W. A. Skoda[3], Robert M. J. Jacobs[4], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Germany — [2]Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Germany — [3]ISIS, RAL, Didcot, UK — [4]CRL, University of Oxford, UK

Liquid-liquid phase separation (LLPS) in protein solutions plays an important role for protein crystallization. Phase diagrams of HSA and BSA with Yttrium Chloride (YCl_3) in the c_p and c_s plane were determined; a reentrant phase behavior [1] was observed. Here, we show that LLPS can be induced in protein solutions by using YCl_3 [2]. Phase boundaries were determined by UV and X-ray absorption. The effective protein-protein interaction upon LLPS was investigated by SAXS. By optical microscopy of the condensed regime the LLPS region was defined by the formation of liquid droplets. In the case of HSA no cluster formation was observed, whereas BSA formed clusters outside and at the LLPS borders. The reduced second virial coefficient B_2/B_2^{HS} for HSA decreased from a slightly negative value in the condensed regime below the critical value of -1.5 in the LLPS region. For BSA, more negative values were observed at the LLPS border than in between. This is consistent with other protein systems studied. LLPS for HSA and BSA by adding YCl_3 and the clustering in BSA solutions can be explained by a sufficient low and negative B_2/B_2^{HS}. [1] F. Zhang et al., PRL 101, 2008, 148101; [2] F. Zhang et al. Soft Matter, submitted.

CPP 22.2 Wed 11:00 Poster A

Anomalous Small-Angle X-ray Scattering (ASAXS) Study of Multi-Valent Cations around Proteins in Solution — •Baohu Wu[1], Fajun Zhang[1], Maximilian W.A. Skoda[2], Robert M.J. Jacobs[3], Michael Sztucki[4], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen — [2]ISIS, RAL, UK — [3]CRL, University of Oxford, UK — [4]ESRF, France

A detailed understanding of the ion environment is essential for a full description of charged protein systems. ASAXS represents a powerful tool for studying the distribution of targeted ions [1]. We studied protein solutions (β-lactoglobulin, BLG) in the presence of Y3+ using ASAXS. Systematic measurements show clearly energy-dependent ASAXS shifts visible in the scattered intensity. The pure anomalous term which is about 0.02% to 0.2% of the total signal for Y3+ has been successfully separated using the matrix method. The number of ions around the protein, which contribute to the ASAXS signal, is between 1 to 6 per BLG dimer depending on the initial concentration of salt and protein. The number increases from 2.4 to 5 with BLG concentration at a fixed ion concentration, which is due to the cluster formed in re-entrant condensation phase regime [2]. These data are compared with our crystallographic study [3], which indicates 2 to 4 Y3+ binding per BLG dimer. The work will contribute to a comprehensive understanding of the role of the ions in protein crystal growth. [1] M. Sztucki, et al. J. Appl. Cryst. 2010, 43, 1479. [2] F. Zhang, et al. Phys. Rev. Lett. 2008, 101, 148101. [3] F. Zhang, et al. J. Appl. Cryst. 2011, 44, 755.

CPP 22.3 Wed 11:00 Poster A

Substrate effects of the substrate on the formation of polyelectrolyte multilayers — •Maximilian Zerball, Chloé Chevigny, and Regine von Klitzing — Stranski-Laboratorium, Institut für Chemie, TU Berlin

For the past twenty years, the Layer-by-Layer technique (LbL) has made it possible to modify surfaces by covering them with thin films. This technique gives the opportunity for a wide variety of potential applications for polyelectrolyte multilayers (PEM), for example chemical reactors, antireflective coatings or microcontainers.

The deposition of PEMs is influenced by various parameters, such as ionic strength, pH value and charge density. But a systematic study of the substrate effect on the PEM is still missing. Especially, for hybrid/composite materials the connection (interphase) between the PEM and a solid material is important. This addresses planar surfaces like metal or semiconductors as substrates, but also solid particles. For this purpose different substrates were studied by directly changing the nature of the substrate (Silicon or Gold), but also by chemical modification of the silicon surface using silanization (change of both substrate charge and interactions with polyelectrolytes). For polyelectrolytes we chose to use the two most widely spread systems, PSS/PAH and PSS/PDADMAC.

The properties of the PEM are monitored after the deposition as a function of the number of layers by a complementary use of ellipsometry (with humidity control) and AFM. The question is, how far and how strong the structure of the PEM is affected by the substrate.

CPP 22.4 Wed 11:00 Poster A

Influence of the surface chemistry on the coexistence of flatly and brush-like physisorbed chains in poly(styrene-sulfonate) layers — •Stephan Block[1], Frank Lawrenz[2], and Christiane A. Helm[2] — [1]ZIK HIKE - Zentrum für Innovationskompetenz Humorale Immunreaktionen bei kardiovaskulären Erkrankungen, Fleischmannstr. 42 - 44, D-17487 Greifswald, Germany — [2]Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Str. 6, D-17487 Greifswald, Germany

AFM with a colloidal probe as a tip is used to measure the surface forces and to image sodium poly(styrene sulfonate) (PSS) layers which are physisorbed to different surfaces in the presence of 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. Interestingly, this coexistence is observed on hydrophobic (e.g. HOPG, silanized silica) as well as hydrophilic surfaces (e.g. PEI on silicon, PAH on mica). The surface forces can be described as a superposition of electrostatic and steric forces, the former originating from the flatly adsorbed PSS and the latter from the brushes. This indicates that a heterogeneous layer structure seems to be a general phenomenon for physisorbed PSS layers and has to be regarded in studies concerning the adsorption behavior of polyelectrolytes.

CPP 22.5 Wed 11:00 Poster A

On the internal structure of polyelectrolyte multilayers — •Malte Passvogel[1], Peter Nestler[1], Olaf Soltwedel[2], Ralf Köhler[3], and Christiane A. Helm[1] — [1]Institut für Physik, Uni Greifswald, Felix-Hausdorff-Str. 6, 17487 Greifswald, Germany — [2]FRM II, Lichtenbergstr. 1, 85747 Garching, Germany — [3]Stranski-Lab, TU Berlin, 10623 Berlin; Institut F-I2, HZB Berlin, 14109 Berlin, Germany

Polyelectrolyte multilayers from PSS and PDADMAC formed in 0.1 M NaCl solution are investigated. With in-situ ellipsometry first exponential, then linear growth is observed. In the linear growth regime, with increasing PDADMAC molecular weight the thickness per deposited PDADMAC layer and thus the thickness per PDADMA/PSS layer pair increase for PDADMAC polymer weight below 100 kDa, then they level off. Qualitatively, the same results are obtained with X-ray reflectivity from films formed with a different number of PSS/PDADMA layer pairs. However, quantitative comparison shows that films in the exponential growth regime shrink much more on drying (ca 55 %) than the thicker films in the linear growth regime (35 %). With neutron reflectivity the position and width of an internal interface between protonated and deuterated blocks is determined. While the position of the internal interface does not move after deposition, the width increases due to interdiffusion. It is smallest next to the film/air interface and increases towards the core zone of the film until an equilibrium value is reached.

CPP 22.6 Wed 11:00 Poster A

Influence of two-dimensional lamellar phase of PSS on the condensed phase of oppositely charged TAP monolayers — •Heiko Ahrens, Thomas Ortmann, Andreas Gröning, Frank Lawrenz, and Christiane A. Helm — Institut für Physik, Uni Greifswald, Felix-Hausdorff-Str. 6, 17487 Greifswald, Germany

Polystryene sulfonate (PSS) is adsorbed from dilute solution (0.01 mM with respect to the monomer concentration) onto oppositely charged TAP lipid monolayers. TAP lipids are 1,2-alkyl-trimethylammonium-propane with different alkyl chains (14, 16, 18). PSS adsorption stabilizes the monolayer and changes alkyl chain order (NNN to NN) in the liquid condensed phase as evidenced by grazing incidence X-ray diffraction (GID). Simultaneously, with GID the two-dimensional lamellar phase of PSS is observed. The rod scans of the peaks attributed to the PSS reveal that the two-dimensional lamellar phase imposes a slight vertical distortion on the lipid monolayer. The combined analysis of electron density profiles measured by X-ray reflectivity and the rod scans allow to assign the scattering centers within the lipid monolayers. The results are consistent for the different alkyl chain lengths.

CPP 22.7 Wed 11:00 Poster A

Polyelectrolyte coupling to a charged lipid monolayer: relating lattice and domain structures — •Thomas Ortmann, Heiko Ahrens, Andreas Gröning, Frank Lawrenz, and Christiane A. Helm — Institut für Physik, Uni Greifswald, Felix-Hausdorff-Str. 6, 17487 Greifswald, Germany

Polystyrene sulfonate (PSS) is adsorbed from dilute solution (0.01 mM with respect to the monomer concentration) onto oppositely charged dioctadecyldimethylammonium bromide (DODAB) lipid monolayers. The PSS molecular weight is varied. With grazing incidence X-ray diffraction (GID) the two-dimensional lamellar phase of adsorbed PSS is observed, when DODAB is in the condensed phase. The same ordered PSS phase is also found when the lipids are in the fluid phase and PSS molecular weight exceeds 6.5 kDa. A large spacing between short stretched chains hinders the two-dimensional lamellar phase, presumably the short chains gain rotational entropy.

With Brewster Angle Microscopy (BAM) the nucleation and growth of domains is observed on clean water, but only when low molecular weight PSS (< 8 kDa) is used. For high molecular weight PSS no domains of DODAB with coupled PSS are found, even though GID indicates the nucleation of condensed lipid domains. The domains do not grow, which is attributed to hindered lipid diffusion due to the adsorbed macromolecules.

CPP 22.8 Wed 11:00 Poster A

AFM characterization of structural changes of polycation covered surfaces induced by hydroxyl radicals — •Florian Berg[1], Stephan Block[2], and Christiane A. Helm[1] — [1]Institut für Physik, Uni Greifswald, Felix-Hausdorff-Str. 6, 17487 Greifswald, Germany — [2]ZIK HIKE, Uni Greifswald, Fleischmannstr. 42 - 44, D-17487 Greifswald, Germany

Positively charged, branched polyethylenimine (PEI) adsorbed onto silicon wafers are attacked by free hydroxyl radicals. AFM is used to image the PEI layers in air. After the radical attack the PEI layers show 1.3nm high plateaus (area fraction 5 %). With Colloid Probe technique, the force profiles between adsorbed PEI layers before and after the radical attack are measured in NaCl solution of different ionic strength. The force profiles of freshly deposited flat PEI layers show that an electrostatic repulsion dominates the interaction. After the radical attack we find both surface potential and surface charge are reduced by a factor of about two, while the Debye length remains unchanged.

Negatively charged colloidal gold nanoparticles are adsorbed onto the oppositely charged PEI. After the radical attack we find a reduction in saturation surface coverage consistent with the decreased surface charge. Additionally, the adsorption kinetics is slowed down suggesting that the PEI-layer is no longer a flat, compact layer.

CPP 22.9 Wed 11:00 Poster A

The effect of a wedge on the ionic distribution of an electrolyte solution — •Dmitriy Rozhkov[1], Sofia Kantorovich[1,2], and Marcello Sega[2] — [1]Ural Federal University, Lenin av 51, 620083, Ekaterinburg, Russia — [2]Institute for Computational Physics, Pfaffenwaldring 27, 70569 Stuttgart, Germany

Nanoscopic confinement of ionic solutions is often met in both biological systems and technical applications. As long as the behaviour of ionic solutions in confinement is not fully understood, computer simulations are often employed to investigate the subject. However, electrostatic effects, which occur due to the presence of interfaces, should be properly allowed for. Here, we present molecular dynamics simulations of monovalent salt confined in a rectangular, charged box which releases counterions into the solution. Different height to width ratios and various salt concentrations are studied.

CPP 22.10 Wed 11:00 Poster A

Effective interactions in electrolyte solutions — •Markus Bier and S. Dietrich — Max-Planck-Institut IS, Stuttgart, Germany

The effective interactions between walls or colloidal particles are known to be significantly influenced by the properties of a liquid medium in contact. Well-known examples are dispersion forces, which are determined by the permittivity, electrostatic forces, which become short-ranged due to the screening of the Coulomb potential by ions, and solvation forces, which arise due to solvent adsorption or desorption. Commonly these contributions to the effective interactions are assumed to be independent, i.e. the effective interactions are expected to be a simple superposition. However, recently experimental observations for a binary liquid mixture containing salt were reported [1] which cannot be understood by assuming solvation forces being uncoupled from the screened electrostatic forces. Here a possible mechanism [2] is discussed in terms of which all experimental evidence can be explained consistently.

[1] U. Nellen, J. Dietrich, L. Helden, S. Chodankar, K. Nygard, J. van der Veen and C. Bechinger, Soft Matter **7**, 5360 (2011).

[2] M. Bier, A. Gambassi, M. Oettel and S. Dietrich, EPL **95**, 60001 (2011).

CPP 22.11 Wed 11:00 Poster A

Influence of charge density on bilayer bending rigidity in lipid vesicles: a combined dynamic light scattering and neutron spin-echo study — •Beate-Annette Brüning[1], Ralf Stehle[1,2], Peter Falus[3], and Bela Farago[3] — [1]Helmholtz Zentrum Berlin, Hahn-Meitner Platz 1, 14109 Berlin, Germany — [2]Universität Bayreuth, Postfach 10 12 51, 95440 Bayreuth, Germany — [3]Institut Laue-Langevin, B.P. 156, 6 rue Jules Horowitz, 38042 Grenoble, France

We report a combined dynamic light scattering and neutron spin-echo study on vesicles composed of the uncharged helper lipid DMPC and the cationic lipid DOTAP. Mechanical properties of a model membrane and the corresponding fluctuation dynamics can be tuned by changing composition. We compare the bilayer undulation dynamics in lipid vesicles composed of DMPC/DOTAP to vesicles composed of DMPC and the also uncharged reference lipid DOPC. We find, that on the local scale, lipid headgroup composition and charge change the vesicle fluctuations less than acyl chain packing inhomogenities between the composite lipids. We discuss this result on the basis of domain formation in the lipid mixtures containing charged (DMPC/DOTAP) and uncharged reference lipid (DMPC/DOPC). First, we investigate lipid vesicle size and mass diffusion using dynamic light scattering, then we study collective bilayer undulations and bulk diffusion on two distinct time scales around 25ns and 150ns, using neutron spin-echo spectroscopy. Finally, we estimate bilayer bending rigidities κ_B for the charged and uncharged lipid vesicles.

CPP 22.12 Wed 11:00 Poster A

Interfacial engineering of polymer multilayers with polarized biomolecules: a new approach in growing supramolecular layer structures — •Neelima Paul[1,2], Amitesh Paul[3], Stephan Mattauch[4], Peter Müller-Buschbaum[2], and Martha Ch. Lux-Steiner[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [3]TU München, Physik-Department, LS Neutronenstreuung, James-Franck-Str. 1, 85748 Garching, Germany — [4]JCNS Forschungszentrum Jülich GmbH Outstation at FRM II Lichtenbergstrae 1, 85747 Garching, Germany

The development of polymer-based structures is hindered due to the difficulties in realizing well-defined modulated structures with very small interlayer roughness out of charged polymers. We compare two types of heterostructures, one of them was prepared with embedded layers of polarized biomolecules. Using specular and off-specular neutron scattering, we observe,in the heterostruture containing the biomolecule, formation of ordered modulated structures with a drastic decrease in the roughness parameter. For the multilayer without the biomolecule we have indications of formation of island-like structures. Our study thus demonstrates that polarized biomolecules can interrupt the propagation of island-like structures at such interfaces which can be effectively used in achieving well defined supramolecular layer structures out of charged polymers.

CPP 22.13 Wed 11:00 Poster A

Charge-Controlled Metastable Liquid-Liquid Phase Separation in Protein Solutions as a Universal Pathway Towards Crystallization — •Felix Roosen-Runge[1], Fajun Zhang[1], Roland Roth[2], Marcell Wolf[1], Maximilian W.A. Skoda[3], Robert M.J. Jacobs[4], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen — [2]Institut für Theoretische Physik, Universität Erlangen-Nürnberg — [3]ISIS, RAL, Chilton, Didcot, UK — [4]CRL, University of Oxford, UK

We demonstrate that a metastable liquid-liquid phase separation (LLPS) can be induced by multivalent metal ions in solutions of globular proteins at room temperature [1]. Importantly, the approach is applicable to proteins, which otherwise show no LLPS in the full accessible temperature range. The ion and protein partitioning in the coexisting phases is determined in solutions of human serum albumin (HSA) and YCl_3. We interpret the finding on the basis of a phase diagram with three control parameters: temperature, metal-ion and protein concentration. The underlying mechanism of specific ion binding is discussed along the lines of charge inversion and reentrant condensation [2,3]. Interestingly, we find protein crystallization close to the metastable LLPS, consistent with theoretical predictions and simulations suggesting a two-step crystallization process. Thus, multivalent ions can be used to control the phase behavior of protein solutions, including metastable LLPS and protein crystallization.

[1] F. Zhang, et al., Soft Matter, submitted; [2] F. Zhang, et al., PRL (2008) 101:148101; [3] F. Zhang et al., Proteins (2010) 78(16):3450-7

CPP 22.14 Wed 11:00 Poster A

Ionic force field optimization and modified ion-pair mixing rules — •Maria Fyta[1] and Roland Netz[2] — [1]Physik Department, Technische Universität München, 85748 Garching, Germany — [2]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany

We propose an optimization scheme to obtain good ionic force fields for classical simulations of salt solutions, also of biological relevance. Our work is based on Molecular Dynamics simulations with explicit water for different halide and alkali ions forming salt solutions at finite ion concentration. The force field derivation technique we propose is based on a simultaneous optimization of single-ion and ion-pair properties and the determination of the cation-anion interaction parameters (traditionally given by the mixing rules). From the finite-concentration simulations, thermodynamic properties of the salt solutions are derived, using the Kirkwood-Buff theory of solutions, and compared to relevant experimental data. For the rather size-symmetric salt solutions involving bromide and chloride ions, this scheme using the standard mixing rules works fine. For the iodide and fluoride solutions, corresponding to the largest and smallest anion we have considered, a rescaling of the mixing rules was necessary. In this respect, we have introduced scaling factors for the cation-anion Lennard-Jones interaction that quantify deviations from the standard mixing rules. We discuss the efficiency and complications of the proposed ionic force field optimization scheme.

CPP 22.15 Wed 11:00 Poster A

Chain conformation of polyelectrolytes at surfaces as deduced from the surface forces — •Stephan Block[1] and Christiane A. Helm[2] — [1]ZIK HIKE - Zentrum für Innovationskompetenz Humorale Immunreaktionen bei kardiovaskulären Erkrankungen, Fleischmannstr. 42 - 44, D-17487 Greifswald, Germany — [2]Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Str. 6, D-17487 Greifswald, Germany

The measurement of force profiles can be used to determine the chain conformation adopted by polymers and polyelectrolytes after deposition to a surface. Usually, for each conformation a characteristic length scale exists which sets the interaction length of the force profile. E.g., the electrostatic interaction usually dominates the surface forces of flatly physisorbed polyelectrolytes in aqueous solution; the characteristic length scale is the Debye length which is controlled by the ionic strength. We show how the scaling of the characteristic length can be used to obtain information about the chain conformation when the ionic strength is varied. Additionally, we apply existing theories to measured force profiles and evaluate their feasibility.

CPP 22.16 Wed 11:00 Poster A

Quasilinear electro-optic effect in ferroelectric polymer-dispersed nematic liquid crystals due to remanent polarization — •Lars Hollänedr, Werner Wirges, and Reimund Gerhard — Universität Potsdam, Institut für Physik und Astronomie, Potsdam

Polymer-dispersed liquid crystal (PDLC) films were prepared using ferroelectric poly(vinylidenefluoride-trifluoroethylene) (P(VDF-TrFE)) and nematic 4-cyano-4-n-hexylbiphenyl (6CB). Inside the composite material the liquid crystal 6CB was separated in discrete micrometer-sized droplets with nearly spherical shape. The transparency change due to an applied external electric field was measured for non-poled and poled samples.

Usually the change in transmittance of nematic PDLC-films depends only on the absolute value of the electric field and not on the polarity. But after the poling of the PDLC device the remanent polarization of the P(VDF-TrFE) creates an internal electric field, which acts as an offset. It is assumed that due to the internal field the preferred orientation of the nematic liquid crystal inside the droplets is changed from a radial to an axial one. This pre-alignment in field direction causes a quasilinear transmittance behavior as well as a general increase of transparency.

CPP 22.17 Wed 11:00 Poster A

Mixtures of Chitosan and Oppositely Charged Alkyl Ethoxy Carboxylates: Complex Hierarchical Structures — •Leonardo Chiappisi[1], Sylvain Prévost[1,2], and Michael Gradzielski[1] — [1]Stranski-Laboratorium für Physikalische Chemie und Theoretische Chemie, Institut für Chemie, Technische Universität Berlin, Berlin, Germany — [2]Helmholtz-Zentrum Berlin, Berlin, Germany

Mixtures of polyelectrolytes and surfactants are widely used in a large number of fields, such as detergency, pharmaceutical formulations, food industry, etc. Their aggregation is driven by several forces, ranging from electrostatic to hydrophobic interaction and mostly by the entropic gain due to the release of counterions from both polymer and surfactant micelles.

Here, we present a comprehensive structural study on mixtures of the biopolycation chitosan and the highly biocompatible alkyl ethoxy carboxylates. In order to elucidate the structure of these complexes, static and dynamic light scattering (SLS and DLS) have been used to explain the large scale structure, whereas small angle neutron scattering (SANS) has been employed to determine the internal structure of the complexes.

The results show that the shape of the micelle is retained within the complex, that they are locally linearly ordered and that the large scale structure is determined by the folding of the polymerchain. In addition, the formation at higher surfactant content of larger and hierarchically ordered structures made up of many polyelectrolyte chains is proven.

CPP 22.18 Wed 11:00 Poster A

Dielectric spectrum of salt solutions from molecular dynamics simulations — •Marcello Sega[1], Sofia Kantorovich[1,2], Axel Arnold[1], and Christian Holm[1] — [1]Institute for Computational Physics, Pfaffenwaldring 27, 70569 Stuttgart, Germany — [2]Ural Federal University, Lenin av 51, 620083, Ekaterinburg, Russia

We present the results of MD simulations for water salt solutions with various salt concentrations. Following the experimental approach, we use several fit-functions in order to determine static dielectric permittivities. We show, that the permittivity obtained via Einstein-Helfand fit is extremely sensitive to the statistics and, as a result is very difficult to use reliably. However, the static value of the dielectric permittivity can be evaluated by fitting the complete frequency-dependent spectrum, using, for example, the Cole-Cole relation. We compare our results to the experimental data from [Buchner et al, J. Phys. Chem. A, Vol. 103, 1999, P. 1], which show an initial linear decrease of the static dielectric permittivity as a function of salt concentration, and a saturation at high concentrations.

CPP 23: Poster: Polymer Dynamics

Time: Wednesday 11:00–13:00 Location: Poster A

CPP 23.1 Wed 11:00 Poster A

Theoretical Investigations of Semiflexible Dendrimers — •Florian Fürstenberg, Maxim Dolgushev, and Alexander Blumen — Theoretische Polymerphysik, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Deutschland

Dendrimers are branched, highly regular synthetic polymers. Here we investigate the mechanical relaxation of semiflexible dendrimers of arbitrary functionality f and generation g. We focus on the matrix corresponding to their potential energy[1] and show that the semi-analytical determination of its (highly degenerate) spectrum can be drastically simplified by using a suitable decomposition scheme[2].

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

[2] F. Fürstenberg, M. Dolgushev, and A. Blumen, to be published.

CPP 23.2 Wed 11:00 Poster A

Simulation of externally stimulated polymer chains — •Kirsten Dammertz, Masoud Amirkhani, and Othmar Marti — Institute of Experimental Physics, Ulm University

In this contribution, we explore by atomistic Molecular Dynamics (MD) simulations the possibility to stimulate and align polymer molecules by electric fields. As model polymers we use various pyridine-containing homopolymers adsorbed on graphite. The primary objective of our study is to investigate conformational changes, dipole reorientations and the trajectory of the molecules. Based on our simulations, we quantify the influence of the chemical composition as well as the strength and orientation of the external field. Polymer-specific conformational characteristics are discussed.

All MD simulations are carried out by means of the LAMMPS software package. To define the potential functions and force field parameters, we apply the polymer consistent force field (pcff).

CPP 23.3 Wed 11:00 Poster A

Controlling adsorption of semiflexible polymers — •Tobias Kampmann and Jan Kierfeld — Technische Universität Dortmund, Deutschland

We investigate the adsorption of single semiflexible polymers on planar and structured substrates. Using Monte-Carlo simulations we determine the critical potential strength for square-well adsorption potentials over a wide range of persistence lengths.

For a planar substrate we find a maximum of the critical potential strength for persistence lengths comparable to the potential range. In the stiff limit, we derive an analytical result, which agrees with the simulation results. We also investigate the influence of an additional surface curvature for adsorption on a sphere and on a ”washboard” surface.

CPP 23.4 Wed 11:00 Poster A

The behaviour of a nanoparticle in a polymer melt — •Anja Kuhnhold and Wolfgang Paul — Institut für Physik, Martin-Luther-Universität, 06099 Halle

The rheology of polymer melts can be observed by looking at the behaviour of suspended particles (microrheology). For this purpose MD simulations of a bead-spring model including one nanoscopic particle are performed. The dynamic behaviour of the nanoparticle is determined by its mean square displacement (MSD) and velocity autocorrelation function (VCF). Using a generalized Stokes-Einstein equation, we observe the complex shear modulus $G^*(\omega)$ of the melt. Furthermore, the influence of different particle sizes, interaction strengths and polymer chain lengths is studied. The results are in agreement with predictions of the Rouse model in the low frequency regime. Additional structural information of the polymer melt in the vicinity of the nanoparticle are given by radial distribution functions (RDFs).

CPP 23.5 Wed 11:00 Poster A

Ring Rotation Dynamics of Ferrocene and Ferrocene-containing Polymers — •Markus Appel[1,2], Bernhard Frick[2], Tinka Spehr[1], and Bernd Stühn[1] — [1]TU Darmstadt (Germany) — [2]Institut Laue-Langevin, Grenoble (France)

Ferrocene is an organometallic compound consisting of two cyclopentadienyl rings with a reversibly oxidizable iron atom sandwiched in between. Bulk ferrocene shows a structural phase transition at 164 K (triclinic to monoclinic). Ferrocene-containing polymers are of high interest for applications in nanotechnology as they combine polymeric with metallic properties and can show ferromagnetic susceptibilities.

As an important aspect of the characterization of ferrocene-containing polymers we study the cyclopentadienyl ring rotation dynamics. We aim to compare the ring rotation of bulk ferrocene to ferrocene contained in polymers using inelastic neutron scattering.

Past neutron scattering studies of the ring rotation dynamics in bulk ferrocene mainly focussed on the high temperature phase [1]. We present neutron time-of-flight and backscattering experiments including the new possibility of inelastic fixed window scans (IFWS) on IN16 at the ILL [2] of the low temperature phase of ferrocene. The extracted correlation times and activation energy of the rotation dynamics are found to be considerably higher than for the high temperature phase.

Additionally, we present first measurements on the ferrocene-containing polymer poly(vinylferrocene).

[1] Gardner et al., Chem. Phys. **57**, 453 (1981)

[2] Frick et al., Nucl. Inst. and Methods A, accepted for publication

CPP 23.6 Wed 11:00 Poster A

Experimental and theoretical study of the yellowing of ancient paper — Adriano Mosca Conte[1], Olivia Pulci[1,2], Arkadiusz Knapik[3], Jacek Bagniuk[3], Joanna Łojewska[3], and •Mauro Missori[4] — [1]ETSF, Dept. of Physics, Università di Roma Tor Vergata, Rome, Italy — [2]Institute of Structure of Matter, National Research Council, Rome, Italy — [3]Faculty of Chemistry, Jagiellonian University, Krakow, Poland — [4]Institute of Complex Systems, National Research Council, Rome, Italy

Paper has been the most widely used writing support since the Middle Ages. The preservation of ancient books and documents must be based on an advanced knowledge of the paper degradation processes. Yellowing causes major damage for the aesthetic appearance of ancient paper and it is due to cellulose oxidation, a complex process with many possible products, some of them chromophores, still to be clarified. In this talk, we will present experimental ultraviolet-visible spectra of ancient papers of the 15^{th} century and, as reference, modern samples artificially aged under different environmental conditions. With the aid of ab-initio Time-Dependent Density Functional Theory calculations, we investigate several possible oxidized forms of cellulose polymers. Through the comparison of measured and calculated optical spectra, we identify those oxidized groups which act as chromophores. Our non-destructive approach could be used as a powerful method to estimate the state of degradation of historical papers and in the research of bleaching and reducing agents to be employed in the restoration practice.

CPP 23.7 Wed 11:00 Poster A

Theoretical aspects of branched semiflexible polymers — •Maxim Dolgushev and Alexander Blumen — Theoretische Polymerphysik, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Deutschland

In recent years the theory of semiflexible polymers has seen advances in the mathematical-analytical study of branched structures[1]. Nowadays one can model semiflexible treelike polymers, in which the branching points may have arbitrary functionality and stiffness[2,3]. A further step forward concerns the investigation of semiflexible polymers containing loops, i.e. obeying closure conditions. The treatment of such objects is rendered possible through the maximum entropy principle[4], as we have recently shown for rings[5].

[1] M. Dolgushev, G. Berezovska, and A. Blumen, Macromol. Theory Simul. 20, 621 (2011)

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

[3] M. Dolgushev and A. Blumen, J. Chem. Phys. 132, 124905 (2010).

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

[5] M. Dolgushev, G. Berezovska, and A. Blumen, J. Chem. Phys. 135, 094901 (2011).

CPP 23.8 Wed 11:00 Poster A

Influence of pressure on deviations of chain dynamics from the Rouse model: A molecular dynamics simulation study of poly(dimethylsiloxane) and polybutadiene melts. — •Patrick Henritzi[1], Dmitry Bedrov[2], Grant Smith[2], and Michael Vogel[1] — [1]Intitut für Festkörperphysik, TU Darmstadt, 64289 Darmstadt, Germany — [2]Department of Material Science and Engineering, University of Utah, Salt Lake City, Utah 84112, USA

Molecular dynamics simulations of poly(dimethylsiloxane) (PDMS) and polybutadiene (PBD) melts have been performed as a function of pressure. At atmospheric pressure the single-chain coherent dynamic structure factor of PBD exhibited greater deviation from ideal Rouse behavior than PDMS, in agreement with neutron spin echo (NSE) measurements. Chain dynamics in both PDMS and PBD exhibited increasing deviations from Rouse predictions with increasing pressure. These deviations were found to correlate with the free volume fraction in the melt, implying that inter-chain correlations and not intrinsic rotational barriers are mainly responsible for non-ideal chain dynamics in polymer melts.

CPP 23.9 Wed 11:00 Poster A

Structure and Dynamics of Polyethylene Glycol Polymer Rings — •Sebastian Goossen[1], Ana Rita Brás[1], Wim Pyckhout-Hintzen[1], Andreas Wischnewski[1], Jürgen Allgaier[1], Dimitris Vlassopoulos[2,3], and Dieter Richter[1] — [1]Jülich Centre for Neutron Science JCNS (JCNS-1) & Institute for Complex Systems (ICS), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]FORTH, Institute of Electronic Structure and Laser, Heraklion, Crete, 71110, Greece — [3]University of Crete, Department of Materials Science and Technology, Heraklion, 71003, Greece

The structural analysis of highly pure polyethylene glycol (PEG) polymer rings in a theta solvent with SAXS and with SANS in the melt showed a significantly more compact structure for the ring polymers compared to their linear equivalents of same molecular weight. The dynamical behavior of ring polymers and linear chains was studied in the melt by NSE spectroscopy. In comparison the ring polymers showed a significantly faster center of mass diffusion than the linear chains. This turns out to be an explicit violation of the Rouse model. Furthermore blends of ring polymers in a matrix of linear polymer chains were investigated with these techniques. For PEG ring polymers with a molecular weight above the entanglement molecular weight Me the observed center-of-mass diffusion in the linear matrix is surprisingly low compared to PEG polymer rings below Me. This leads to the question if, due to the interpenetration of ring polymers and linear polymer chains, collective diffusion occurs in these blends.

CPP 23.10 Wed 11:00 Poster A

Intimate coupling of heterogeneous dynamics and structural relaxation independent of molecular weight, temperature, and pressure. — •André Bormuth and Michael Vogel — Hochschulstraße 6, 64289 Darmstadt

Performing molecular dynamics simulations for an all-atom force field, we study the segmental or, equivalently, α relaxation of poly(propylene oxide) chains consisting of $N = 2 - 100$ monomer units. In particular, we analyze the dependence of the α relaxation time τ_α on molecular weight, temperature, and pressure on the basis of incoherent intermediate scattering functions. Regarding dynamical heterogeneities, we monitor the non-Gaussian parameter and the weight-averaged mean cluster size. Both quantities exhibit a maximum for intermediate times, where the peak height and the peak time τ_p increase upon cooling and pressurizing. Interestingly, we find that data for different chain length, T, and p collapse onto a single Master curve $\tau_p = a * \tau_\alpha^b$, suggesting a close relation between structural relaxation and spatially heterogeneous dynamics. The exponent b turns out to be the same for the non-Gaussian parameter and the weight-averaged mean cluster size, indicating evidence for an underlying basic principle. Using the coupling model from Ngai et al. we discuss a way of tracing back the Parameters a and b to physical quantities.

CPP 23.11 Wed 11:00 Poster A

Weakly Segregated Polymers in Electric Fields — •Christian W. Pester[1], Markus Ruppel[2], Volker S. Urban[3], and Alexander Böker[1] — [1]DWI an der RWTH Aachen and Lehrstuhl für Makromolekulare Materialien und Oberflächen, RWTH Aachen, D-52056 Aachen, Germany — [2]Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN 37831, USA. — [3]Neutron Scattering Science Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN 37831, USA.

We elaborate on the effects of electric fields on weakly phase separated block copolymers in non-selective solvents. In a series of theoretical papers E. Gurovich proposed the reorientation of individual copolymer chain segments due to the external stimulus. The resulting anisotropic distortion of chain conformations results in orientation-dependent alterations of gyration radii with respect to the electric field vector. The resulting anisotropic character of correlation holes is expected to have a profound effect on the small-angle scattering patterns. Indeed, in-situ synchrotron small-angle X-ray scattering (SAXS) at the ESRF in Grenoble allowed us to identify some of the theoretically predicted consequences these elliptical gyration radii would have on the scattering signal, i.e. on domain spacings and order-disorder transitions.

CPP 23.12 Wed 11:00 Poster A

Light-induced deformation of amorphous azo-polymers: structure-property relation — Vladimir Toshchevikov[1], Jaroslav Ilnytskyi[2], and •Marina Saphiannikova[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany — [2]Institute for Condensed Matter Physics, Lviv, Ukraine

Recently, we have proposed a microscopic theory [1] of light-induced deformations in amorphous side-chain azo-polymers. The theory is able to predict a sign of the sample deformation (contraction/elongation) depending on angular distributions of chromophores in respect to the backbone. For instance, it is shown that an azo-polymer demonstrates a uniaxial elongation along the polarization vector of the light, if azobenzenes are attached to a stiff backbone and have preferable orientation perpendicular to it. This kind of behavior has been indeed observed in molecular dynamics simulations of azo-polymers with short spacers [2]. The present contribution is aimed to relate quantitatively the theoretical and simulation studies by feeding certain structural properties obtained in the simulations into a theory input. Especially, the backbone rigidity and angular distribution of chromophores have been studied at different light intensities and temperatures. This work may open a way for fine tuning of photomechanical properties of azo-polymers by modifying their chemical structure.

This work was supported by the DFG grant GR 3725/2-1.

[1] V.Toshchevikov, M.Saphiannikova, G.Heinrich. J. Phys. Chem. B 2009, 113, 5032; [2] J. Ilnytskyi, D. Neher, M. Saphiannikova. J. Chem. Phys. 135, 044901 (2011).

CPP 23.13 Wed 11:00 Poster A

Two - point Nanorheology based on single molecule FRET in polymer PMA — •subhasis adhikari, markus selmke, and frank cichos — Molecular Nano-photonics, Inst. of Expt. Phys I, University of Leipzig

Fluorescence Resonance Energy Transfer (FRET) has been widely used in structural biology, biochemistry and in polymer science to measure the distances in very short range (2nm - 10nm) depending on the donor - acceptor pair. To study the heterogeneous dynamics in polymers near its glass transition temperature (Tg) a new technique, Two-point Nanorheology based on FRET is used in single molecule optical studies. This study will reveal the rheological information of the local environment surrounding the dye molecules at a nanometer length scale by measuring distance fluctuations. Firstly Alexa 488 (donor) and then Alexa 594 (acceptor) are attached to amino - thiol terminated polystyrene polymer by a standard synthesis and characterized by fluorescence methods.The single donor dye labeled polymer aggregates in DMF but not in toluene as detected by Fluorescence Correlation Spectroscopy (FCS) technique. Ensemble FRET and single molecule FRET (smFRET) are measured and compared to each other. The reorientation factor is calculated from fluorescent anisotropy studies.

CPP 23.14 Wed 11:00 Poster A

Filling process in cylindrical nanopores — •Manuela Lukas and Bernd Stühn — Experimentelle Physik kondensierter Materie, TU Darmstadt, Germany

The aim of this work is to investigate the filling flow behavior of polymers in nanopores using time resolved Small-Angle X-ray Scattering (SAXS). The nanoporous samples consist of a polycarbonate foil with thickness 30 μm, irridated with swift heavy ions (ion tracked polycarbonate: ITPC), treated with UV light and etched in NaOH solution. Varying the etching time the cylinder radii can be controlled. In ITPC nanopores are aligned strictly parallel. For filling experiments polydimethylsiloxane (PDMS) with three different molecular weights, (M=28,000 g/mol, M=63,000 g/mol, M=139,000 g/mol), is used. PDMS was chosen because its electron density with $\rho = 319e/nm^3$ is different to the electron density of the matrix material polycarbonat with $\rho = 380e/nm^3$ showing a good contrast for SAXS. The filling process is shown by the steady decrease in scattering intensity with time. It turns out that the intensity variation with time follows the Lucas-Washburn equation. The $\sqrt{t}$ -dependency of the filling height is reproduced well throughout the whole filling process. However a quantitative analysis of the full scattering profiles reveals a remarkable deviation from the classical filling behaviour [M. Engel, B. Stühn. *J. Chem. Phys.* 132, 224502, 2010]. Furthermore the data suggest the forming of a precursorfilm.

CPP 23.15 Wed 11:00 Poster A

Specific vs. unspecific interaction and aggregation in bulk supramolecular polymers — •Tingzi Yan[1], Klaus Schröter[1], Florian Herbst[2], Wolfgang Binder[2], and Thomas Thurn-Albrecht[1] — [1]Institute of Physics, Martin-Luther University Halle-Wittenberg — [2]Institute of Chemistry, Martin-Luther University Halle-Wittenberg

Hydrogen bonded supramolecular polymers have attracted much attention in the past decade due to their special properties. They combine the advantages of polymers and of non-covalently bonded supramolecules with reversible structures. In general, the association behavior in solution is simpler and better understood than in the bulk. We present combined small angle x-ray scattering and rheological experiments, complemented by IR spectroscopy on a series of polyisobutylene chains terminated with hydrogen bonding units of different strengths. While in solution the functional units form specific bonds, SAXS measurements in the bulk for all samples show partially ordered structures and large aggregates, indicative of additional demixing between the PIB chains and the functional groups. Hydrogen bonds obviously stabilize these aggregates, even at high temperatures as it is shown by IR spectroscopy. The rheological properties which vary strongly between different samples and depend strongly on temperature, result from the combined effect of supramolecular interaction and additional structure formation. The specificity on the hydrogen bonds seems to be lost in the bulk sample.

CPP 24: Poster: Organic Semiconductors

Time: Wednesday 11:00–13:00 Location: Poster A

CPP 24.1 Wed 11:00 Poster A

Plasmonics in nanostructured organic solar cells — •Thomas Pfadler[1], Ricky Dunbar[1], and Lukas Schmidt-Mende[2] — [1]LMU Munich — [2]University of Konstanz

Organic solar cells have the potential to become an important low-cost alternative to conventional solar cells. However, before this can happen, the energy harvesting potential of organic solar cells must become more comparable with that of the pervading technology. This research is based upon the construction of organic solar cells that demonstrate highly favourable light-plasmonic coupling at a nanostructured silver electrode. These nanostructured silver electrodes are prepared via nanoimprint lithography (NIL) and optimised to improve the light harvesting and efficiency of organic thin-film solar cells. Given appropriate control of loss mechanisms such as interfacial recombination, the absorption enhancement will correspond to an increase in the solar cell efficiency.

CPP 24.2 Wed 11:00 Poster A

Ortho- and Terminal-substituted Perylene Diimides as Acceptor Materials for Organic Solar Cells — •Valentin Kamm, Glauco Battagliarin, Ian A. Howard, Michael Hansen, Hans W. Spiess, Chen Li, Klaus Müllen, and Frédéric Laquai — Max-Planck-Institute for Polymer Research, Mainz, Germany

Perylene diimide (PDI) is a promising electron acceptor material for high open circuit voltage bulk heterojunction organic solar cells. However, many PDI molecules have the tendency to strongly aggregate leading to intermolecular excited state formation that can result in exciton trapping.[1] Recently, a method for substitution at the ortho-position of the PDI core was introduced giving access to novel acceptor molecules.[2] The substitution affects the stacking and therefore the charge carrier mobility and excited state energies and dynamics. In this contribution we present the excited state and intermolecular packing of a series of PDI molecules with different substitution patterns at the terminal- and ortho-position investigated by time-resolved photoluminescence and solid-state NMR techniques.

[1] I. A. Howard, F. Laquai, P. E. Keivanidis, R. H. Friend, N. C. Greenham, J. Phys. Chem. C, 2009,113, 21225-21232. [2] Glauco Battagliarin, Chen Li, Volker Enkelmann, and Klaus Müllen, Organic Letters, 2011,13,3012-3015.

CPP 24.3 Wed 11:00 Poster A

Photophysical Characterisation of Novel Polymeric Absorber Materials for Organic Solar Cells — •Hannah Mangold[1], Ian A. Howard[1], Ralf Mauer[1], Silvia Janietz[2], and Frédéric Laquai[1] — [1]MPI for Polymer Research, Mainz, Germany — [2]Fraunhofer IAP, Potsdam, Germany

The power conversion efficiency of organic solar cells has significantly increased in the last year as the old benchmark poly(3-hexylthiophene) (P3HT) has been surpassed by novel donor-acceptor polymers with enhanced absorption in the near-infrared region of the solar spectrum. We investigate terpolymers synthesized with different contents of dialkyl substituted diphenyl-benzopyrazine or diphenyl-thienopyrazine, which determine the optical properties of the materials, and triphenylamine units that should determine the charge transport properties of the material by acting as the hole conductor. Using ultrafast transient absorption we see that the hole indeed transfers to the triphenylamine unit, validating the approach of simplifying material property optimization by decoupling the role of light absorption and hole transport within a single polymer backbone. We achieve open circuit voltages approaching 1V and power conversion efficiencies of 3%, demonstrating the potential of this class of terpolymer. However, the inclusion of the triphenylamine unit does not enhance device performance, and based on light intensity dependent measurements, we attribute this observation to an increase in carrier trapping. Therefore, we demonstrate that it is possible to achieve independent control of light absorption and transport properties with the three monomers of a terpolymer.

CPP 24.4 Wed 11:00 Poster A

Photophysical investigation of core-enlarged rylene dyes for solid state dye-sensitized solar cells — •Yoojin Kim, Michael Meister, Ian A. Howard, Belinda Nölscher, Glauco Battagliarin, Denis Andrienko, Chen Li, Klaus Müllen, and Frédéric Laquai — MPI for Polymer Research Mainz

Perylene derivatives used as sensitizers in solid state dye-sensitized solar cells have attracted a lot of interest owing to their high molar extinction coefficients and broad absorption spectra. However, their absorbance is limited to the visible spectral region. By enlarging the perylene core with additional naphthalene units, the absorption can be extended to the near infrared region. However, devices employing such core-enlarged rylene dyes and an anhydride as anchoring group do not necessarily show higher efficiencies. In this study, the photophysical properties of rylene films in device structures are examined using quasi steady-state photoinduced absorption (PIA) and time-resolved photoluminescence spectroscopy. In presence of the hole transporter Spiro-MeOTAD, we observe a Stark effect in the PIA that suggests a change in the direction of the dipole moment unfavorable for charge separation. This change most probably originates from ring opening of the anhydride group during adsorption to the metal oxide, which is also supported by first-principles (TD-DFT, B3LYP) calculations. However, we note that moderate charge generation and regeneration of the dyes are still observed. By relating our results to solar cell performance we point out the factors which reduce the performance after the spectral response is extended to the infrared region.

CPP 24.5 Wed 11:00 Poster A

Impedance measurements on organic solar cells based on DIP and C_{60} — •Theresa Linderl, Stefan Grob, Julia Wagner, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Impedance spectroscopy (IS) has turned out to be a powerful tool to study organic semiconductor devices by measuring differential resistances and capacitances. Recently, it was shown that a connection can be established between recombination and series resistances extracted from IS and current-voltage (j-V) curves of polymer solar cells [1]. IS bypasses the influence of the photocurrent, which is assumed to be constant and measures directly the recombination current, that in turn can be used to understand the shape of the j-V curve of a solar cell. In this contribution we apply this method to describe organic solar cells based on diindenoperylene (DIP) and the fullerene C_{60}. By comparing results of IS measurements of planar- and bulk-heterojunction solar cells we investigate the effect of charge carrier recombination on organic solar cell performance.

[1] P. P. Boix et al., Adv. Eng. Mater. 1 (2011) 1073.

CPP 24.6 Wed 11:00 Poster A

Structural, morphological and electrical characterization of organic donor-acceptor photovoltaic cells based on diindenoperylene (DIP) and C_{60} — •Mark Gruber[1], Monika Rawolle[2], Julia Wagner[1], Alexander Hinderhofer[3], Andreas Opitz[4], David Magerl[2], Jan Perlich[5], Stephan V. Roth[5], Frank Schreiber[3], Peter Müller-Buschbaum[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg — [2]TU München, Physik Department, Garching — [3]Fakultät für Physik, Universität Tübingen — [4]Institute of Physics, Humboldt University, Berlin — [5]HASYLAB at DESY, Hamburg

Due to a variation of the substrate temperature during film deposition, the structure and morphology of DIP and C_{60} layers are changed perceptibly. Atomic force microscopy (AFM) images reveal larger lateral grains of both materials for elevated substrate temperatures. With grazing incidence small angle X-ray scattering (GISAXS) measurements we can show that the mean lateral domain distance within the volume of the DIP film increases in the same way as the surface grain size. The vertical domain size of DIP is determined by X-ray diffraction (XRD) measurements, pointing towards coherently ordered domains with a height corresponding to the whole DIP layer thickness. C_{60} on top of DIP forms domains which are twice as large for an increase of substrate temperature during evaporation from room temperature to 100 °C. To demonstrate the effect of enhanced crystallization on planar and planar-mixed organic solar cells, we characterized comparable devices utilizing DIP as donor and C_{60} as acceptor.

CPP 24.7 Wed 11:00 Poster A

Contact and injection properties of organic planar heterojunction solar cells studied by transient current methods —

•Lena Reichardt, Ulrich Hörmann, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Contact properties and charge carrier injection behavior of organic planar heterojunction solar cells have been investigated by means of complementary transient current methods. Charge extraction by linearly increasing voltage (CELIV) at different initial DC bias and impedance spectroscopy (IS) reveal that, depending on the contact properties, injection either of both charge carrier types at the same time or of one type prior to the other one may occur. This corresponds to the injection behavior of poly(3-hexylthiophene)/fullerene (P3HT/C_{60}) and P3HT/diindenoperylene (P3HT/DIP), respectively with PEDOT:PSS and BCP/Al as contacts. Both CELIV and steady state measurements on P3HT/C_{60} directly indicate injection currents in forward direction. By contrast, measurements on P3HT/DIP result in transient current signals of CELIV measurements at bias voltages where no injection current is seen in steady state measurements. The presence of injected charges in both cases is confirmed by IS which exhibits a change in device capacitance with bias voltage. The ability to deliberately influence the presence of injected charges by contact modification might be helpful to determine the mobility of a specific charge carrier type by (dark) CELIV or to prevent unfavorable injection under forward bias in photo-CELIV measurements.

CPP 24.8 Wed 11:00 Poster A

Characteristics of the excitonic processes in molecular donor/acceptor bilayers — •A.K. Topczak[1], A. Steindamm[1,2], M. Brendel[1], P. Schütz[1], and J. Pflaum[1,2] — [1]Exp. Phys. VI, Julius-Maximilians-University Würzburg, D-97074 Würzburg — [2]ZAE Bayern e.V., D-97074 Würzburg

Knowledge of the exciton transport in molecular thin films is of great importance for organic photovoltaic (OPV) applications. We address this issue by Photoluminescence (PL)-Quenching measurements on the molecular semiconductor Diindenoperylene (DIP) in combination with different acceptor (C_{60}, Phthalocyanine) and excitonic blocking (BPhen) materials both of relevance for OPV devices. This technique yields detailed information on the exciton diffusion length, which can be significantly enhanced for highly crystalline materials, and on the exciton dissociation probability at suited donor/acceptor interfaces. As will be demonstrated the latter strongly depends on the respective material combination in correlation with interface morphology and trap states. Furthermore, DIP-PL variation can be attributed to exciton dissociation, recombination or reflection at the respective interfaces. For the case of DIP/C_{60} bilayers, the dissociation efficiency amounts to 90% rendering recombination losses in this bilayer structure almost negligible. To further enhance charge carrier generation in DIP/C_{60} bilayer cells the impact of a BPhen exciton blocking layer was analysed via PL-measurements. By this approach effects by metal penetration and exciton reflection on exciton harvesting and therefore on the macroscopic device performance can be discriminated.

CPP 24.9 Wed 11:00 Poster A

Femtosecond Transient Absorption Spectroscopy of PTB7/PCBM Blend Systems — •Benjamin Müller[1], Björn Gieseking[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — [2]Bavarian Centre for Applied Energy Research (ZAE Bayern), D-97074 Würzburg

Due to their low fabrication costs bulk heterojunction organic solar cells show great potential for photovoltaic applications. The actual certified well working solar cell comprised of the copolymer PTB7 and $PC_{71}BM$ acceptor reaches an efficiency of more than 7% reflecting the remarkable progress in this field [1]. However, recent studies indicate that the device performance strongly depends on the morphology of the active layer and is very sensitive to sample preparation [2].

In this work we investigate the influence of solvent additive on the photophysical properties of PTB7:$PC_{71}BM$ blend films by applying picosecond timeresolved photoluminescence spectroscopy and femtosecond transient absorption spectroscopy. The experimental results are discussed in terms of the influence of the morphology on exciton diffusion and charge carrier photogeneration.

[1] Liang et al., Advanced Energy Materials 2010, 22 [2] Chen et al., Nano Letters 2011, 11, 3707-3713

CPP 24.10 Wed 11:00 Poster A

Open-Source-Code for Numerical Drift-Diffusion Simulations of Organic Solar Cells — •Janine Fischer, Wolfgang Tress, Karl Leo, and Moritz Riede — IAPP, TU Dresden

Organic photovoltaics have recently made impressive progress by reaching efficiencies up to 10%. The versatility of the accessible materials demands for simulation tools explaining and predicting material properties that allow for a specific donator/acceptor synthesis. Numerical drift-diffusion-simulations have repeatedly shown to well reproduce experimental data and provide a powerful tool for the interpretation of measured J-V-curves. Here, we present an open-source-code for device-simulations of multilayer - bulk as well as planar heterojunction - organic solar cells. Our C++-based algorithm iteratively solves the discretized differential equation system comprising the continuity equations for electrons and holes, drift and diffusion currents, as well as the Poisson equation for space-charges caused by free charge-carriers and localized ionized dopants. In particular it also deals with non-linearities introduced by effects such as the field and/or temperature dependence of the mobility, different recombination mechanisms, or various trap distributions which can each be selected individually according to the device design. Additionally, automated parameter variations are enabled.

CPP 24.11 Wed 11:00 Poster A

Polyethylene induced structural modification in polymer blends used in photovoltaic cells — •Ammara Akhtar, Eva M. Herzig, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

Photovoltaic cells consisting of organic semiconducting polymer poly(3-hexylthiophene) (P3HT): fullerene derivative PCBM blends have attracted much interest over the last two decades. In order to improve the morphology of organic materials in solar cells, a third component such as the commodity polymer polyethylene can be introduced. It is reported that among different commodity polymers, high density polyethylene (HDPE) is a promising material for organic solar cells because of an observed improvement in the photocurrent generation efficiency of the system [1]. Furthermore, it is also expected that, the use of HDPE instead of low density polyethylene (LDPE) provides a better control to the microstructure in the final photovoltaic cell because of its highly crystalline nature [2]. In order to improve the interfacial morphology of the P3HT:PCBM blend by adding HDPE spin coating at elevated temperature is necessary. A structural analysis of the ternary system is being carried out with the aid of spectroscopy and scattering experiments. [1] Ferenczi et al., Adv. Mater. 23, 4093 (2011) [2] Goffri et al., Nat.Mater. 5, 950 (2006)

CPP 24.12 Wed 11:00 Poster A

The morphology of flexible all polymer solar cells — •Weijia Wang[1], Matthias A. Ruderer[1], Ezzeldin Metwalli[1], Shuai Guo[1], Kai Scherer[1], Stephan V. Roth[2], Jan Perlich[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany

The interest in photoactive polymers and its applications in organic photovoltaics increased in the last decades dramatically due to promising properties such as mechanical stability, light weight, easy processibility and low cost compared to traditional inorganic solar cells. There have been already many studies on organic solar cells, but only little attention has been focused on fully flexible organic solar cells so far. Carbon nanotubes (CNT) are among the most promising candidates of flexible electrode materials, which can be deposited on flexible PET substrates. In this work, CNT/PET substrates are used as electrodes for solar cells. The CNT/PET substrates are characterized with transmission and resistance measurements. The substrates are coated with an electron blocking layer PEDOT:PSS which is modified by methanol to better wet the substrate. The morphology of the PEDOT:PSS layer is investigated with grazing incidence small angle X-ray scattering and atomic force microscopy methods and its thickness is measured with X-ray reflectivity.

CPP 24.13 Wed 11:00 Poster A

Influence of PSS on the Morphology of P3HT:PCBM Solar Cells — •Anna Naumann, Eva M. Herzig, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

In organic photovoltaics the combination of poly(3-hexylthiophene) (P3HT) and PCBM for the active layer is very promising, but there are still many attempts for further improvement of device efficiency. One approach is to add a third component, like in this case polystyrenesulfonate (PSS), which can increase the performance by almost 30% compared to the reference P3HT:PCBM-cell [1]. PSS is an ionomer, which is neither conductive nor absorbent, hence it has to influence the morphology of the P3HT:PCBM-blend. In our study we analyze the film surface and the crystallization behavior of spin-coated thin films with different mixing ratios with the aid of optical microscopy, atomic force microscopy and x-ray diffraction, respectively. Furthermore, the interaction between substrate and film is of great interest, so an investigation of accumulation layers in the blend is made with reflectivity measurements.

[1] Kim et al. Solar Energy Materials and Solar Cells, 92:1188 (2008)

CPP 24.14 Wed 11:00 Poster A

Comparing the device performance of organic light-emitting diodes processed from solution — •Benedikt Stender[1], Maximilian Nothaft[2], Jörg Wrachtrup[2], and Jens Pflaum[1,3] — [1]Experimental Physics VI, Julius-Maximilian-University of Würzburg, D-97074 Würzburg — [2]3rd Physics Institute and Research Center SCoPE, University of Stuttgart, D-70550 Stuttgart — [3]ZAE Bayern, D-97074 Würzburg

The feasibility of inkjet-printing offers great advantageous in terms of reduced recombination losses and controlled positioning of solution processed organic light-emitting-diodes (OLEDs). However, due to inherent effects of droplet formation and the sensitivity on printing conditions, it still remains challenging to obtain films of similar quality as from spin-coating. For this purpose, the device performance of poly(para-phenylene-vinylene) OLEDs prepared by spincasting and inkjet printing is compared with respect to structural and opto-electronic characteristics. As we will demonstrate, by choosing suited sets of preparation parameters, inkjet printed PPV-OLEDs of similar performance can be achieved, thereby paving the way towards innovative devices based on local doping of the emission layer with single molecules.

CPP 24.15 Wed 11:00 Poster A

Excitonic lifetime changes in organic light-emitting diodes induced by triplet-polaron-quenching — •Sebastian Wehrmeister, Tobias Daniel Schmidt, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Although organic light emitting diodes (OLEDs) have matured in technical applications in recent years they still have not reached high efficiencies. The external quantum efficiency (EQE) and thereby the luminous efficacy is limited by multiple effects, such as low outcoupling efficiency, energy dissipation to surface plasmons and waveguided modes, unbalanced charge carrier ratio and quenching induced non-radiative energy losses especially at high brightness. However, to distinguish between triplet-triplet-annihilation and triplet-polaron-quenching, the two major quenching processes at high brightness, time-resolved measurements under combined electrical and optical excitation have been performed [1]. In our experiments we examine the effect of triplet-polaron quenching on excitonic lifetimes in a phosphorescent OLED with fac-tris(2-phenylpyridine)iridium(III) ($Ir(ppy)_3$) as emitter. We probe exciton lifetime in the steady-state region of a rectangular electric pulse by a short laser pulse on top. In order to achieve reliable data we have continuously increased the current density of the electrical pulse resulting in an exponential decrease of the excitonic lifetime and thus a decrease in the EQE.

[1]N.C. Giebink, S.R. Forrest, Phys. Rev. **B**,235215-1 (2008)

CPP 24.16 Wed 11:00 Poster A

Microscopic charge transport simulations in P3HT lamellae and P3HT:PCBM blends — •Carl Poelking and Denis Andrienko — Max Planck Institute for Polymer Research, Mainz, Germany

Atomistic force fields for poly(3-hexylthiophene) (P3HT) and phenyl-C61-butyric acid methyl ester (PCBM) are parametrized using first-principles calculations. Lamellae of regioregular and regiorandom P3HT are then simulated using atomistic molecular dynamics. Microscopic simulations of charge transport in the resulting morphologies help to identify origins of energetic disorder leading to a different Poole-Frenkel behavior of regiorandom and regioregular P3HT. The role of polarization effects on the relative energy level alignment is then assessed for a P3HT:PCBM blend. Finally, we discuss the impact of energetic disorder on formation of a charge transfer state and efficiency of a P3HT:PCBM bulk heterojunction solar cell.

CPP 24.17 Wed 11:00 Poster A

In situ structural and electrical studies of P3HT droplet solidification — Linda Grodd, •Eduard Mikayelyan, Ullrich Pietsch, and Souren Grigorian — Solid State Physics, University of Siegen, Siegen, Germany

Due to it's good semiconducting properties poly(3-hexylthiophene) (P3HT) is a promising candidate for organic field effect transistors (OFETs). Thus, there is a lot of effort to understand a conduction mechanism and to tune the material properties to receive optimal performance of the final device.

In our studies we investigated the structural and electrical properties of P3HT during the solidification process from the solution to the thin film formation stage. P3HT/chloroform solution was dropped onto Si/SiO_2 substrates with source/drain electrodes to which a fixed voltage was applied. During solidification the structure was investigated by monitoring the (100) reflection and (020) reflection, respectively, using grazing incidence x-ray diffraction (GIXD). Simultaneously, the source/drain current was recorded.

Interestingly, the measurements revealed that the current was peaking just before the Bragg peak intensity had reached its final maximum at the constant level. This fact leads to the conclusion that not only crystalline order, represented by Bragg peak intensity, but the overall network connection is a key parameter for high conductivity.

We gratefully acknowledge the BMBF, Germany for financial support.

CPP 24.18 Wed 11:00 Poster A

Change of unit cell during the growth of Diindenoperylene (DIP) on polycrystalline gold followed by Grazing Incidence X-ray Diffraction — •Sebastian Bommel[1,2], Christopher Weber[2], Peter Schäfer[2], and Stefan Kowarik[2] — [1]HASYLAB at DESY, Notkestr. 85, 22607 Hamburg, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

Organic-inorganic semiconductor hybrid-structures are promising candidates for applications in opto-electronics, photovoltaics and sensing. The molecular structure at the organic-inorganic interface is crucial for the effectiveness of such devices. Here we report results of real-time and in situ grazing incidence X-Ray diffraction (GIXD) measurements for growth of the organic semiconductor diindenoperylene (DIP) on polycrystalline gold. By monitoring the evolution of unit cell we find that the cell parameters a, b, c and the angle beta change during growth. These unit cell changes are a strong indication of a change in molecular tilt for the molecular layers adjacent to the gold surface.

CPP 24.19 Wed 11:00 Poster A

Organic Heteroepitaxy of RGB Nanoneedles — •Martin Oehzelt[1], Clemens Simbrunner[2], Günther Schwabegger[2], Francesco Quochi[3], Ingo Salzmann[4], Antje Vollmer[1], Norbert Koch[1,4], and Helmut Sitter[2] — [1]HZB-BESSY II, Berlin, Germany — [2]Inst. Semincond. and Solid State Physics, JKU Linz, Austria — [3]Dipartimento di Fisica, Universita di Calgiary, Italy — [4]Institut für Physik, HU-Berlin, Germany

Self-assembly processes and organic-organic heteroepitaxy are powerful techniques to obtain highly ordered molecular aggregates. Here we demonstrate that combining both methods allows not only to fabricate highly crystalline and uniaxially oriented self-assembled nanofibers but also to tune their polarized emission. We show that submonolayer coverage of sexithiophene on top of para-sexiphenyl nanofibers is sufficient to change their emission color from blue to green. Triband emission in the red, green, and blue is generated in nanofibers with thicker sexithiophene coverage, where layers of co-oriented crystals are separated by green-emitting molecular sheets. The nanofibers were grown on a dielectric substrate mica and therefore the study of the electronic structure with photoemission is hampered due to sample charging. To solve this problem the same organic heterostructures were grown on HOPG (highly oriented pyrolytic graphite), as evidenced by x-ray diffraction as well as fluorescence measurements. The main difference, however, is that the fibers are not uniaxially oriented any more. Nevertheless, the color-tuning ability and also the crystal plane that makes contact to the substrate surface are preserved on HOPG when compared to mica.

CPP 24.20 Wed 11:00 Poster A

The influence of meso-phenyl torsion on the chemical properties of porphyrine — •Michal Wojdyr, Wichard Beenken, Erich Runge, and Martin Presselt — TU Ilmenau, Ilmenau, Germany

Extension of the porphyrin π-system due to meso-substitution [1] leads to significant changes in the chemical behaviour of porphyrine: porphyrine as well as tetra-mesity-porphyrine can be protonated in a two-step mechanism, while only a one-step mechanism is observed if the meso-positions are bearing phenyl substituents rather than hydrogens or mesityl-groups. Only in case of phenyl substitution the π-system is extended. Therefore, the observed change in basicity may be attributed to electronic effects. However, the torsion of the phenyl against the porphyrine macrocycle induces torsion in the macrocycle too, which also might raise basicity of the porphyrine. To get deeper insights into the dependence of porphyrine basicity on π-conjugation and steric effects, various molecular properties were studied in dependence of the phenyl torsion of mono-protonated porphyrine bearing the phenyl group at one meso-position.

CPP 24.21 Wed 11:00 Poster A

Tuning the light induced charge separation in Ru(II) terpyridine complexes: a quantum chemical study — •Jakob Kreismann, Lars Winterfeld, Erich Runge, and Martin Presselt — TU Ilmenau, Ilmenau, Germany

Ru(II) poly-pyridine complexes have proven their ability to act as photocatalysts, e.g., for the production of molecular hydrogen. One of the essential steps there is the initial charge transfer (CT) transition oxidizing Ru and reducing the ligand sphere, while recombination to the initial ground state should be minimized to maximize the efficiency of further charge transfer to a catalytic active site. In our study, we focus on the dependence of the initial CT on the electronic properties of the terpyridine ligands, which are bearing differently functionalized phenylens at the 4*-position. Using resonance Raman spectroscopy and density functional theory, we found that the CT extends to the functionalized phenylens even at the Franck-Condon point.

CPP 24.22 Wed 11:00 Poster A

Optics and electronic excitations in organic copper complexes from first-principles theory — •Martin Rohrmüller and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn, 33098 Paderborn, Germany

Binuclear Cu complexes play an important role in the enzymatic oxidation and are of potential interest for industrial redox processes [1]. However, the physics and chemistry of the corresponding charge transfer mechanism are not yet fully understood. In order to contribute to a microscopic understanding of the charge and structural dynamics in such complexes we focus on the experimentally well characterised model systems μ-η^2:η^2-peroxodicopper(II) species (P) and the bis-μ-oxodicopper(III) species (O) [2].

We calculate the ground state as well as the optical response and electronic excitations of $[Cu_2(dbdmed)_2(O_2)]^{2+}$ using (Time Dependent) Density Functional Theory and Many Body Perturbation Theory [3]. Particular attention is paid to the influence of the physical and numerical approximations (basis set, exchange-correlation functionals, spin structure) as well as the impact of environment (ligands, solvents).

[1] Solomon *et al.*, Chem. Rev. 1996, **96**, 2563

[2] Mahadevan *et al.*, J. Am. Chem. Soc. 2000, **122**, 10249

[3] Onida *et al.*, Rev. Mod. Phys. 2002, **74** , 601

CPP 24.23 Wed 11:00 Poster A

Vibronic spectra of Frenkel excitons in a 2-dimensional polyacene lattice — •Peter Reineker[1], Ivan J. Lalov[1,2], and Thomas Hartmann[1] — [1]Institute for Theoretical Physics, Ulm University, 89069 Uln, Germany — [2]Faculty of Physics, Sofia University, Sofia 1164, Bulgaria

The vibronic spectra of Frenkel excitons (FEs) in a 2-dimensional lattice which models the (ab)-plane of polyacenes have been studied. The linear optical susceptibilities of the 2-dimensional crystal have been calculated using the Green functions method and the vibronic approach for the spectral ranges of FEs and their vibronic replicas. In the simulations of the vibronic spectra we use the excitonic and vibrational parameters of the crystals anthracene, tetracene and pentacene and obtain the linear absorption spectra in the excitonic and vibronic regions (FE plus one or several intramolecular vibrational quanta). The linear FE-phonon coupling is strong enough to create a bound or quasi-bound state of FE and one phonon, but it is not sufficient to bind the FE and more than one phonon. A hypothetical quadratic FE-phonon coupling makes the bound FE-phonon states more pronounced in the vibronic spectra. The strong transfer of the FE between two sublattices of the polyacene crystals widens the vibronic absorption lines.

CPP 24.24 Wed 11:00 Poster A

A quantum chemical study of the dependency of absorption properties on meso-substituent conformations of two different corrole NH-tautomers — •Philipp Keck, Wichard J. D. Beenken, Erich Runge, and Martin Presselt — TU Ilmenau, Ilmenau, Germany

Corroles, contracted tetrapyrrolic macrocycles lacking one meso-carbon atom, have emerged as attractive porphyrinoid materials for novel catalysts, antitumor treatment and imaging agents as well as active materials in the design of new sensors and optoelectronic devices. We are focussing on the dependency of the optical properties on meso-substituent conformations of two different tautomers, which were spectroscopically distinguished recently. Therefore, extensive density functional theory studies were performed employing the functional BP86 in conjunction with the "multipole accelerated resolution of the identity" approximation to achieve a linear scaling of the computational effort on the system size.

CPP 24.25 Wed 11:00 Poster A

Influence of the treatment of organic films on the blinking dynamics of embedded inorganic QDots — •Ines Trenkmann[1], Harald Graaf[2], and Christian von Borczyskowski[1] — [1]Chemnitz University of Technology, Institute of Physics, Germany — [2]Kassel University, Institute of Chemistry and Center for Interdisciplinary Nanostructure Science and Technology, Germany

The possibility of tailoring properties of hybrid optoelectronic devices, such as light-emitting devices, by embedding inorganic quantum dots (QDots) in organic materials arouse more and more interest in the last years. Mainly the modification of optical properties of QDots due to interactions with the surrounding organic matrix is studied at the ensemble level.

At the same time, single particle studies of QDots reveal fluctuations of the emission intensity. This fluorescence intermittency, mostly denoted as blinking, is commonly explained by trapping of generated charges in the QDots shell and/or surrounding [1]. Only a few studies have analyzed the influence of an organic matrix on the optical properties of single inorganic QDots [2].

In this contribution, we show the variation of the optical properties of CdSe/ZnS-QDots embedded in thin TPD films. Thereby the focus lies on the influence of the film treatment on the blinking dynamics of single QDots and possible effects on the analytics of hybrid optoelectronic devices.

[1] C. Krasselt, et al. PCCP 2011, 13, 17084.

[2] H. Huang, et al. Nano Letters 2007, 7, 3781.

CPP 24.26 Wed 11:00 Poster A

The influence of voltage bias on charge carrier generation and recombination processes in oligothiophene-based organic solar cells — •Christian Koerner[1], Hannah Ziehlke[1], Roland Fitzner[2], Egon Reinold[2], Peter Bäuerle[2], Karl Leo[1], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik, TU Dresden, Dresden, Germany — [2]Institute of Organic Chemistry II and Advanced Materials, University of Ulm, Ulm, Germany

Dicyanovinyl end-capped oligothiophenes (DCVnT) have demonstrated their ability of achieving high power conversion efficiencies of up to 7.0% in a bulk heterojunction solar cell. Additionally, they act as an excellent model system to investigate the influence of systematical changes to the molecular structure on the thin film properties.

We use a sexithiophene derivative to investigate the influence of voltage bias on the charge generation and recombination processes in bulk heterojunction solar cells. Therefore, we combine the normal IV measurement with photoinduced absorption (PIA) spectroscopy. Using this method, we can investigate the long-living (μs-ms) excited species present after photoexcitation of DCV6T:C60 blends acting as photo-active layers in complete and working devices. With PIA, the generation and recombination behaviour of charged molecular states (polarons) are subsequently investigated for various voltage bias and illumination intensities.

CPP 24.27 Wed 11:00 Poster A

Influence of intermolecular gap and film morphology on the open circuit voltage of organic heterojunction solar cells — •Ulrich Hörmann[1], Julia Wagner[1], Mark Gruber[1], Andreas Opitz[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, Germany — [2]Institute of Physics, Humboldt University of Berlin, Germany

The efficiency of a photovoltaic cell is directly proportional to its open circuit voltage. This in turn is eventually set by the intermolecular gap, i.e. the energy of the donor-acceptor charge-transfer state in organic solar cells. In this contribution we introduce diindenoperylene (DIP) as a new molecular acceptor and compare it to C_{60} in planar heterojunction cells. Being able to deliberately change the morphology of the molecular films by varying the substrate temperature during the growth process, we demonstrate that the V_{oc} not only scales with the intermolecular gap but also strongly depends on the morphology of the organic films. We show that planar heterojunctions of thiophene derivatives and DIP yield extraordinarily high open circuit voltages of approximately 1.2 V for poly(3-hexylthiophene) and almost 1.4 V for heat treated α-sexithiophene [1]. Those values are close to the maximum V_{oc} attainable for these material systems.

[1] U. Hörmann *et al.*, phys. stat. sol. RRL 5 (2011) 241

CPP 24.28 Wed 11:00 Poster A

Triplet Exciton Formation and Electron Back Transfer in High-Efficiency Conjugated Polymer-Fullerene Blends studied by Optically Detected Magnetic Resonance — •Hannes Kraus[1], Stefan Väth[1], Andreas Sperlich[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg, Germany — [2]ZAE Bayern, D-97074 Würzburg, Germany

The properties of forward and backward electron transfer between (D)onor and (A)cceptor moieties of polymer-fullerene BHJ solar cells, are vital to the photovoltaic performance. The forward electron transfer is the essential part of efficient charge generation, while its backward counterpart can lead to formation of excitonic states with lower energy (e.g. triplet excitons, TE), culminating in complete loss of the excitation for power generation. We investigated the TE formation attributes of P3HT:PC_{60}BM and P3HT:Lu_3N@PCBEH, finding no triplets in the former, while the latter shows a distinct TE yield. This is conclusive with the relative positions of the energy levels of triplet excitons located on the polymer and the fullerene LUMO. To generalize this assumption, we investigated the D-A blends with different donor polymers and acceptor fullerenes using the optically detected magnetic resonance (ODMR), a method sensitive to the spin state and orientation of quasi-particles. The highly performing PTB7:PC_{70}BM was found to also exhibit both CT and triplet states, whereas P3HT:PC_{70}BM shows only CT state generation. We discuss these findings regarding the morphology and energy level driven electron back transfer.

CPP 24.29 Wed 11:00 Poster A

Charge transport and recombination dynamics in low-bandgap polymer:fullerene solar cells — •Andreas Zusan[1], Andreas Baumann[2], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), D-97074 Würzburg

In the class of low-bandgap conjugated polymers PCPDTBT blended with PC_{70}BM is a promising candidate on the route towards highly efficient organic photovoltaics. The substitution of the bridging carbon atom by silicon (Si-PCPDTBT) is known to cause the formation of separated donor and acceptor phases and an enhanced power conversion efficiency. In this context the transport and recombination dynamics in PCPDTBT:PC_{70}BM and Si-PCPDTBT:PC_{70}BM bulk heterojunction solar cells were studied by the use of charge extraction by linearly increasing voltage (CELIV) under working conditions. We found an enhanced density of photogenerated charges as well as an increased effective charge carrier lifetime for Si-PCPDTBT:PC_{70}BM. The results are explained by the changes in morphology and can be directly linked to the raised device performance bridging the gap between nanoscale and application.

CPP 24.30 Wed 11:00 Poster A

Triplet excimer emission in CBP-derivatives — •Alexander Rudnick[1], Sebastian Hoffmann[1], Pamela Schrögel[2], Peter Strohriegel[2], and Anna Köhler[1] — [1]Uni Bayreuth, Experimentalphysik II — [2]Uni Bayreuth, Makromolekulare Chemie I

Carbazole-biphenyl-derivatives (CBP) are widely used as host matrix materials for efficient phosphorescent organic light-emitting diodes (OLEDs). For blue phosphorescence, a key requirement is a high energy of the triplet excited state, and no other decay channels. Here we have investigated the electronic and optical properties of two series of CBP derivatives using time-resolved fluorescence and phosphorescence measurements in combination with density functional calculations. We show that such materials form sandwich-type triplet excimer states at 2.5 eV that compete with the monomer triplet state at 3.0 eV and that are detrimental to OLED performance.[1] The broad excimer emission can be suppressed using three approaches, (i) by adding sterically demanding outer groups, (ii) by enforcing torsion of the central biphenyl group and (iii) by changing the position where the pendant carbazole is attached to the biphenyl moiety from a para- to a meta-connection.[2,3]

[1]ST Hoffmann et al, J. Phys. Chem. B, 2011, 115, 414-421
[2]P. Schrögel et al, J. Mater. Chem., 2011, 21, 2266-2273
[3]P. Schrögel et al, Organic Electronics, 2011, 12, 2047-2055

CPP 24.31 Wed 11:00 Poster A

Correlation between polymer architecture, mesoscale structure and photovoltaic performance in PAE-PAV:fullerene bulk-heterojunction solar cells — •S. Rathgeber[1], F. Kühnlenz[2], H. Hoppe[2], D.A.M. Egbe[3], S. Türk[4], J. Perlich[5], and R. Gehrke[5] — [1]University Koblenz-Landau — [2]Ilmenau University of Technology — [3]Johannes Kepler-University Linz, Austria — [4]Chemnitz University of Technology — [5]DESY.

A poly(arylene-ethynylene)-alt-poly(arylene-vinylene) (PAE-PAV) statistical copolymer carrying linear and branched alkoxy side chains along the conjugated backbone in a random manner, yields, compared to its regular substituted counterparts, an improved performance in polymer:PCBM bulk-heterojunction solar cells. GiWAXS experiments show that the improved performance of the statistical copolymer may be attributed to the following structural features: 1. Well, ordered stacked domains that promote backbone planarization and thus $\pi\pi$-overlap. 2. Partly face-on alignment of domains relative to the electrodes for an improved active layer electrode charge transfer. Branched side chains seem to promote face-on domain orientation. They might minimize their unfavorable contact with the interface by just bringing the CH_3 groups of the branches into direct contact with the surface so that favorable phenylene-substrate interaction can promote face-on orientation. 3. A more isotropic domain orientation throughout the active layer i.e. the backbone alignment direction has components perpendicular and parallel to the electrodes compromises between light absorption and intra-chain charge transport.

CPP 24.32 Wed 11:00 Poster A

Optical characterisation of highly ordered donor-acceptor films as fabricated by means of the Langmuir Blodgett technique — •Felix Herrmann[1], Sviatoslav Shokhovets[1], Harald Hoppe[1], Uwe Ritter[1], Rainer Beckert[3], Karl-Heinz Feller[2], Gerhard Gobsch[1], Erich Runge[1], and Martin Presselt[1] — [1]TU Ilmenau, Ilmenau, Germany — [2]University of Applied Sciences Jena, Jena, Germany — [3]Friedrich Schiller Universität, Jena, Germany

In organic solar cells the interface between electron donor and acceptor molecules is of crucial importance for charge separation, but is rather inhomogeneous and difficult to characterize in bulk-heterojunction organic solar cells. Therefore, we applied the Langmuir-Blodgett technique to tune the molecular ordering at the heterointerface of donor-acceptor bilayers up to more or less crystalline phases. The applied substances need to possess an amphiphilic structure to realize high surface pressures. As donor we used [6,6]-phenylC61-butyric acid and as donor a highly photostable thiazole derivative. The optical properties of these devices are characterizes by means of photothermal deflection and photoluminescence spectroscopy.

CPP 24.33 Wed 11:00 Poster A

Effect of doping on bias stress behavior of organic thin-film transistors — •Moritz Hein, Alexander Zakhidov, Moritz Riede, and Karl Leo — IAPP, TU Dresden

During the last few years, organic thin-film transistors have taken many important steps on their way into the market. By now they already reached a performance level that allows contributions in first applications such as backplanes for E-Ink-displays. An important problem regarding is the stability of the transistors during permanent gate bias stress. If the transistor operates on constant voltages for a longer period of time, the current flow between source and drain electrode is continuously reduced. This reversible degradation is found to be caused by a transport of charge carriers from the accumulation channel into the dielectric of the transistor and depends on the energy levels of both the dielectric and semiconductor. Hence, we compare the bias-stress effect for different organic semiconductors with given transistor geometry and silicon dioxide as dielectric material. Also we investigate the behavior of the characteristic transistor parameters before and after the bias-stress treatment. For the example of the system MeO-TPD on silicon dioxide, we show how the amplitude of the bias-stress effects can be reduced by weak doping of the semiconductor and a thereby induced shift of the Fermi energy.

CPP 25: Poster: Stress Relaxation in Polymers - From single molecules to biological cells (joint focus with BP)

Time: Wednesday 11:00–13:00 Location: Poster A

CPP 25.1 Wed 11:00 Poster A

Influence of the microstructure on the viscoelastic behavior of thin films of polypropylenes — •Martin Neumann, Toni Hille, and Robert Magerle — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

With a microtensile testing setup that allows for simultaneous imaging with atomic force microscopy (AFM) we correlate the changes of the microstructure occurring during aging and deformation processes with the viscoelastic behavior of thin films of semicrystalline polymers. We study elastomeric polypropylenes (ePP) with different degrees of crystallinity (12% to 40%) and different molecular weights polymerized with metallocene catalysis. The films were annealed for several hours at different temperatures, which results in different microstructures and in turn different types of stress strain behavior and stress relaxation phenomena. For ePP films the elastic moduli are in the range between 0.2 and 10 MPa and the relaxation times between 2 s and 100 s. Cyclic loading experiments show changes of viscoelastic properties that are attributed to aging and crystallization processes. Series of AFM images measured at increasing strain show the deformation of individual lamella in spherulites in thin films of polypropylene with ultra-high molecular weight and 99% tacticity. At large deformations fractures and crazing between spherulites are observed.

CPP 25.2 Wed 11:00 Poster A

Characterization of conformational changes of single-chain, thin film and bulk polymers — •Frank Zocholl[1], Massimiliano Labardi[2], Daniele Prevosto[2], Kirsten Dammertz[1], Masoud Amirkhani[1], and Othmar Marti[1] — [1]Institute of Experimental Physics, University of Ulm, 89069 Ulm, Germany — [2]Dipartimento di Fisica Enrico Fermi, Università di Pisa, Largo Pontecorvo 3, 56127 Pisa, Italy

The possibility to induce conformational changes in Poly(4-Vinylpyridine) (P4VP) by application of ambient gas or electric fields is investigated. Characterization of dielectric properties both in bulk and thin films of P4VP are carried out by dielectric spectroscopy techniques, to find information about glass transition temperature and relaxation processes. Broadband Dielectric Spectroscopy (BDS) is a well established technique for dielectric study of bulk samples. Local Dielectric Spectroscopy (LDS) is a new approach based on Atomic Force Microscopy (AFM), applicable to ultra-thin films and capable of high spatial resolution, by sensing electric forces between the sample and the AFM tip. By means of a customized setup, shifts in instantaneous resonance frequency of the force sensor due to an ac applied voltage are measured, and provide information on the dielectric function of the material. By measuring dielectric relaxation dynamics for various thicknesses it is possible to evidence the effects of both spatial confinement and presence of interfaces.

CPP 25.3 Wed 11:00 Poster A

Synthesis and spectroscopic characterization of BODIPY dyes with aliphatic substituents in polymer matrices — •Melanie Bibrach, Stefan Krause, Christian von Borczyskowski, and Robert Magerle — TU Chemnitz, Fakultät für Naturwissenschaften, D-09126 Chemnitz

Boron dipyrrin (BODIPY) derivates are popular dyes for single molecule spectroscopy because of their high photoefficency and photostability. We aim at using BODIPY labelled polymers as fluorescent probes for the macromolecular dynamics in polypropylene and other semicrystalline polymers that is caused by relaxation of mechanical stress. To this end we synthesized BODIPY derivates with aliphatic substituents of different length from precursor molecules via the Heck reaction. Here we report on their spectroscopic characterization on the ensemble level. The fluorescent probes were embedded in thin films of different polymers (polypropylenes, block copolymers). Fluorescence spectra and fluorescence lifetime were measured in the temperature range from -50 °C to 160 °C. We discuss our results with respect to structural and dynamic changes of the polymers, such as glass transition and cystallisation.

CPP 25.4 Wed 11:00 Poster A

Computer simulation study of viscoelastic properties of entangled polymers using a translationally invariant slip-spring model — •Veronica Chappa[1,2], David Morse[3], Annette Zippelius[2], and Marcus Müller[2] — [1]CONICET, Argentina — [2]Institut für Theoretische Physik, Georg-August-Universität, Göttingen, Germany — [3]Department of Chemical Engineering and Materials Science, University of Minnesota, USA

Different slip-spring models have been proposed and used to describe the behavior of entangled polymers in computer simulation. Some of them break translational invariance by anchoring slip-links to fixed points in space or alter the equilibrium properties of the polymeric chains. We introduce a slip-spring model that represents entanglements via pairwise, translationally and rotationally invariant interactions and exactly compensate for the additional interactions such that the presence of slip-springs does not modify the equilibrium statistics of the polymers. These slip-springs were implemented in computer simulations of a soft coarse-grained polymer model and we study the viscoelastic properties of entangled polymer systems. Each end of a slip-spring can move to a neighboring segment along the chain to which it is attached and renewal processes at chain ends simultaneously account for tube renewal and the effect of constraint release. We present results for the mean squared displacements, shear viscosity, stress relaxation, and diffusion of the slip-springs along the chains in equilibrium and under flow. Our simulation results are compared to theoretical models and experiments.

CPP 25.5 Wed 11:00 Poster A

Changes in Structural and Wetting Properties of Polyelectrolyte Multilayers upon Mechanical Load — Johannes Früh[1], Adrian Rühm[2], Helmuth Möhwald[1], Rumen Krastev[3], and •Ralf Köhler[4,5] — [1]MPIKG Potsdam, Interfaces, 14424 Potsdam/Golm — [2]MPIMR Stuttgart, ZWE FRM II, 85747 Garching — [3]NMI at the University of Tübingen, Biomaterials, 72770 Reutlingen — [4]TU Berlin, Stranski-Lab, 10623 Berlin — [5]HZB, Soft Matter (F-I2), 14109 Berlin; Germany

Polyelectrolyte Multilayers (PEM) are formed by alternating adsorption of oppositely charged organic macromolecules onto a charged template. Despite big attempts for understanding the complex interactions in PEM and their subsequent effects, several major features are still unclear. This study addresses the mechanical properties of thin PEM films, with focus on the molecular changes upon lateral stress. Internal and overall restructuring is investigated using neutron and X-ray reflectivity, and UV-vis spectroscopy. An transition from elastic to plastic deformation is observed at an elongation of ca 0.2%. (A very tiny value which resembles the behaviour of solid bodies.) The transition is attended by, either a reversible, or an irreversible uptake of water from the ambient atmosphere. A superstructure created by selective replacing of PSS with deuterated PSS in the PSS/PDADMAC-multilayer showed gradual and irreversible degradation of the layer structure upon elongation. Decoiling of entangled polymer chains which, in extra, are strongly interacting via ionic bonds is considered as the origin of the molecular intermixing upon mechanical load.

CPP 25.6 Wed 11:00 Poster A

"Stress relief" via embedding of cyclopropane derivatives in polymers — •Miriam Wollenhaupt and Dominik Marx — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum

Due to their special physical properties such as elasticity, breaking strength, chemical and thermal stability, polymers are widely used. But continuous strain causes weakening of the polymer strands and, therefore, leads to material failure. The embedding of mechanophores (stress-responsive chemical groups that undergo a chemical reaction when exposed to a mechanical force) in the single polymer chains can provide a "stress relief".

Under mechanical forces, gem-dichlorocyclopropanes incorporated along the backbone of cis-polybutadiene exhibit an electrocyclic ring opening accompanied with a chlorine migration[1].

Besides the practical aspects, theoretical investigations on cis- and trans-1,1-dichloro-2,3-dimethylcyclopropane unveil a field of striking features, such as a lack of selectivity at high forces or unexpected branching ratios[2]. We used static calculations to investigate the change of electronic properties along the reaction pathways under different forces. The analysis of wavefunction and electron density was performed using Natural Bond Orbitals and Quantum Theory of Atoms In Molecules.

[1] J. Am. Chem. Soc., 2009, 131, 10818–10819

[2] Angew. Chem. Int. Ed., 2011, 50, 7105–7108

CPP 25.7 Wed 11:00 Poster A

Güte der Abstandsmessungen von D-Banden in Kollagenfibrillen — •Christopher Robert Pech[1] und Robert Magerle[2] — [1]Fakultät für Mathematik, TU Chemnitz, D-09107 Chemnitz — [2]Fakultät für Naturwissenschaften, TU Chemnitz, D-09107 Chemnitz

Mittels Rasterkraftmikroskopie ist eine mikroskopische Untersuchung des lokalen Deformationsverhaltens von Kollagenfibrillen in Sehnen und Bänder möglich [1]. Noch gibt es aber keinen Algorithmus und eine dazugehörige umfassende Analyse, die den Abstand zwischen zwei benachbarten D-Banden und den dabei gemachten Fehler bestimmt. Bisher wird über die Gesamtheit mehrerer Abstände gemittelt [1]. Wir entwickeln daher einen Algorithmus, der über die einzelnen Pixel interpoliert und dann den Abstand zwischen benachbarten lokalen Extrema bestimmt. Dieser Algorithmus wird an verschiedenen Testproblemen erprobt, um die Genauigkeit sowie die Störanfälligkeit bei verschiedenen Arten von Rauschen zu bestimmen. Der Algorithmus soll eingesetzt werden, um Veränderungen des lokalen Deformationsverhaltens von Kollagenfibrillen in chemisch behandelten Sehnen zu untersuchen, die als Transplantate eingesetzt werden.

[1] S. Rigozzi et al., J. Struct. Biol. **176**, 9 (2011)

CPP 25.8 Wed 11:00 Poster A

Ultrastructure and the viscoelastic properties of anterior cruciate ligament studied with atomic force microscopy — •Mandy Göring[1], Eike-Christian Spitzner[1], Stephanie Röper[1], Anke Bernstein[2], and Robert Magerle[1] — [1]Chemische Physik, TU Chemnitz, D-09107 Chemnitz, Germany — [2]Department für Orthopädie und Unfallchirugie, Muskuloskelettales Forschungslabor, Universitätsklinikum Freiburg, D-79106 Freiburg, Germany

Tears of the anterior cruciate ligament (ACL) are one of the most common injuries in young and active humans. In today's surgical practice, it is common to use autologous graft tissue for ACL reconstruction. Allografts have recently gained popularity in orthopaedic sports medicine, especially in primary and revision reconstruction of ACL. However the allografts need to be sterilized either by freeze-drying, with peracetic acid or gamma radiation. Most current sterilization procedures have inherent disadvantages affecting biological properties and mechanical function of the graft. We investigate cryosections and collagen fibres isolated from bovine ACL. The samples are prepared like human grafts, adsorbed onto a silicon wafer and studied with atomic force microscopy (AFM) operating in tapping mode. The local viscoelastic properties of the specimen are determined by measuring the dissipated energy between the AFM tip and the collagen fibril as well as the local indentation of the tip into the surface. Changes of the ultrastructure and local viscoelastic properties are discussed with respect to the different types of chemical and physical treatment.

CPP 25.9 Wed 11:00 Poster A

Modeling the stretch and relaxation properties of cytoskeletal filament systems in neutrophil — •Othmar Marti[1], Michael Beil[2], and Stephan Paschke[3] — [1]Institute of Experimental Physics, Ulm University, D-89081 Ulm — [2]Department of Medicine, University Hospital Ulm, D-89081 Ulm — [3]Department of Surgery, University Hospital Ulm, D-89081 Ulm

The individual contribution of cytoskeletal filament systems to the regulation of cell deformation remains to be elucidated in detail. We investigated the mechanical behavior of differentiated NB4 cells which are a model for neutrophil granulocytes [1]. Cellular deformability was studied by optical stretching [2] before and after cells were exposed to cytochalasine D and colchicine to disassemble the actin cytoskeleton and microtubules, respectively. The mechanical response of the cells in the stretcher was modeled by a mechanical model consisting of parallel and series connections of elastic and viscous elements. We found that the salient features of the deformation curves can be described adequately. Microtubules were discovered to mainly contribute to cell elasticity, whereas filamentous actin was in control of cell viscosity in this model system. This link between the cytoskeleton and cell mechanics might point to novel options for the pharmacological modulation of the cell migration.

[1] Bruel, A., Paschke, S., Jainta, S., Zhang, Y., Vassy, J., Rigaut, J.P. and Beil, M., Anticancer. Res. 21, 3973-80 (2001) [2] Guck, J., Ananthakrishnan, R., Mahmood, H., Moon, T.J., Cunningham, C.C. and Käs, J. , Biophys. J. 81, 767-84 (2001).

CPP 25.10 Wed 11:00 Poster A

Conformational properties of stretched and unstretched semiflexible polymer chains — •Hsiao-Ping Hsu[1], Wolfgang Paul[2], and Kurt Binder[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany — [2]Theoretische Physik, Martin Luther Universität Halle-Wittenberg, von Seckendorffplatz 1, 06120 Halle, Germany

Semiflexible polymer chains under good solvent conditions are described by self-avoiding walks on the square and simple cubic lattices in $d = 2$ and $d = 3$ dimensions, respectively, and the stiffness of chains is controlled by the bending energy ϵ_b. With the pruned-enriched Rosenbluth method (PERM), we observe a double crossover behavior, rigid-rod-like to (almost) Gaussian random coils, then to self-avoiding walks, for the chain length up to $N = 50000$ in $d = 3$, but only a single crossover from rigid-rod-like to self-avoiding walks for the chain length up to $N = 25600$. in $d = 2$. Testing the applicability of the Kratky-Porod model, we also check whether the chain conformation is dominated by the excluded volume effects or not as the chain length and its flexibility vary. We extend our study to the problem of stretching semiflexible chains. Varying the strength of the force, the flexibility of the chain, and the chain length, the theoretical predictions of the force-extension relationship at different length scale regimes (linear response - Pincus blob - Kratky-Porod model - freely joined chain) are checked. Our large scale Monte Carlo simulations give clear evidence for the importance of excluded volume effects on the stretching behavior of semiflexible polymer chains.

CPP 25.11 Wed 11:00 Poster A

The effect of moisture on mechanical deformation of PETG — •masoud amirkhani[1], Andrew Boryor[2], Juliana Kurniadi[3], Martin Geiger[2], Thanapon Panchapongsaphak[2], Othmar Marti[1], and Bernd Lapatki[2] — [1]Institute of Experimental Physics, University of Ulm, Germany — [2]Department of Orthodontics, University of Ulm, Germany — [3]DWI at RWTH Aachen e.V. and ITMC / TexMC, RWTH Aachen University, Germany

In this work, we studied the deformation properties of polymer systems in the presence of the water molecules. Depending on the type of polymer network, water molecule may cause softening or hardening of the network. This study shows that polyethylene terephthalate (PETG) immersed in water initially swells whereby its stiffness decreases but after a certain time its stiffness increased to almost its initial point as shown in Figure 1. We applied three-point bending experiments on several stripes (10mm x 55mm) of PETG immersed in water for 14 days. The experiments showed that the elastic modulus of the tested PETG material decreases until 30 hours, after which a gradual increase in the elastic modulus was experienced until 14 days where the E-module almost reached that of the dry material. The reduction of the elastic modules is due to plasticiser effect, which is caused by dispersing water molecules in the network. The increase in stiffness after 30 hours can be attributed to the rearrangement of the polymer chain which also causes a repelling of the water molecules from the polymer network.

CPP 26: Poster: New Perspectives of Scattering at Soft Matter

Time: Wednesday 11:00–13:00 Location: Poster A

CPP 26.1 Wed 11:00 Poster A

Structural evolution in diblock copolymer thin films with perpendicular lamellar structure during solvent vapor treatment

— •Jianqi Zhang[1], Alessandro Sepe[1], Richard Steinacher[1], Jan Perlich[2], Dorthe Posselt[3], and Christine Papadakis[1] — [1]TU München, Physikdepartment, Physik weicher Materie, Garching, Germany — [2]HASYLAB at DESY, Hamburg, Germany — [3]Roskilde University, IMFUFA, Denmark

Well-ordered structures formed by self-assembly of diblock copolymer have attracted increasing interest due to the potential applications. However, the usual preparation methods often result in defects which hamper the application. Vapor treatment with solvents is a commonly used technique to anneal defects in thin films. We have investigated the structural changes of lamellae-forming P(S-b-B) diblock copolymer thin films with perpendicular lamellar structure using in-situ, real-time grazing-incidence small-angle X-ray scattering with a time resolution of 30 s. Cyclohexane and ethyl acetate were used for vapor treatment, which are selective for PB and PS, respectively. We have found that new narrow Bragg rods appear before the diffuse Bragg rods bend in the vapor. These findings point to an initial formation of a thin near-surface layer having the perpendicular orientation and a later destabilization of the perpendicular orientation. The main reason is the change of chain conformations, i.e. a tendency to coiling of the initially stretched copolymers upon solvent uptake.

CPP 26.2 Wed 11:00 Poster A

Diffusion of proteins in a bicontinuous microemulsions: A combined fluorescence correlation spectroscopy and neutron spin echo study

— •Ralph Neubauer, Sebastian Höhn, Christoph Schulreich, and Thomas Hellweg — Phys. und Biophys. Chemie (PC III), Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany

In bicontinuous microemulsions (ME) the oil and water components form sponge-like domains which are separated by a surfactant/co-surfactant film. This structure shows two dynamics: Bulk diffusion (water and oil domain) and film diffusion (surfactant), which can be observed by dynamic light scattering (DLS), neutron spin echo (NSE) and fluorescence correlation spectroscopy (FCS).

For FCS the label determines the type of diffusion which will be observed. Using an amphiphilic fluorescent molecule the diffusion of the surfactant film can be measured. By choosing a fluorescent apolar protein the movement of this particle in the water domain is detected and the confinement effect can be identified. In NSE experiments the deuteration decides about what is measured. If one component in the ME is protonated and the remaining components are matched out by deuteration, only the diffusion of the protonated component is analyzed. When all four components are deuterated and a protein (is inserted in the water phase, the diffusion of the protein will be obtained, also leading to a indepent information about the confinement effect in a ME.

CPP 26.3 Wed 11:00 Poster A

A SANS study of 'patchy' worm-like surface-compartmentalized nanostructures

— •Frank Lüdel[1], Sabine Rosenfeldt[2], Joachim Schmelz[3], Ludger Harnau[4], Thomas Hellweg[1], and Holger Schmalz[3] — [1]Physical and Biophysical Chemistry III, University of Bielefeld, Germany — [2]Physical Chemistry I, University of Bayreuth, Germany — [3]Macromolecular Chemistry II, University of Bayreuth, Germany — [4]MPI for Intelligent Systems, Stuttgart, Germany

A very promising way towards hierarchically self-organized nanostructures is provided by the crystallization-induced self-assembly of polymers [1-3]. Currently, there is only a partial understanding of a few structures with patch-like surfaces having different compartments. Worm-like micelles with a core-corona structure from a semi-crystalline triblock terpolymer (SEM) in organic media were prepared [1]. Its soluble corona exhibits a patchy structure of microphase-separated polystyrene (S) and poly(methyl methacrylate) (M) enclosing a crystalline polyethylene (E) core. The structure formation is triggered by crystallization during cooling. SANS measurements with contrast variation were performed on a SEM with deuterated S-blocks (dSEM) for studying the structure in solution. Results thereof confirm a compartmentalized structure and are presented in this contribution.

[1] Schmalz, H.; Schmelz, J.; et. al. Macromolecules, 2008, 41, 3235.
[2] Schmelz, J.; et al. ACS Nano, 2011, in print; DOI:10.1021/nn202638t
[3] Tang, Z.; Kotov, N. A. Adv. Mater., 2005, 17, 951.

CPP 26.4 Wed 11:00 Poster A

Subsurface influence on the structure of protein adsorbates revealed by *in situ* X-ray reflectivity

— •Hendrik Hähl[1], Florian Evers[2], Samuel Grandthyll[1], Peter Loskill[1], and Karin Jacobs[1] — [1]Saarland University, Experimental Physics, D-66041 Saarbrücken — [2]Condensed Matter Physics Laboratory, Heinrich Heine University Düsseldorf, D-40225 Düsseldorf

The adsorption process of proteins to surfaces is governed by the mutual interactions between proteins, solution and substrate. Interactions arising from the substrate are usually attributed to the uppermost atomic layer. This "actual surface" defines the surface chemistry and hence steric and electrostatic interactions. For a comprehensive understanding, however, also the interactions arising from the bulk material have to be considered.

High energy X-ray reflectivity measurements enable the *in situ* determination of the density profile of the formed protein film. The results of these experiments clearly reveal the influence of the subsurface material on the adsorbing proteins via van der Waals forces. Thereby, the used set of functionalized silicon wafers enables a distinction between effects of the surface chemistry and the subsurface composition of the substrate: Whereas the surface chemistry controls whether or not the individual proteins are denatured, the strength of the van der Waals forces affects the final layer density and hence the adsorbed amount of proteins. The results imply that van der Waals forces mainly influence surface processes, which govern the structure formation of the protein adsorbates, such as surface diffusion or spreading.

CPP 26.5 Wed 11:00 Poster A

The P03/MiNaXS beamline at PETRA III: new opportunities for advanced SAXS/WAXS microbeam in-situ experiments using synchrotron radiation

— •Stephan V. Roth[1], Adeline Buffet[1], Ralph Doehrmann[1], Sebastian Gogolin[1], Mottakin Abul Kashem[1], Gerd Herzog[1], Jan Perlich[1], Matthias Schwartzkopf[1], and Gunthard Benecke[1,2] — [1]DESY, Notkestr. 85, D-22607 Hamburg, Germany — [2]MPIKG Golm, Abt. Biomat., Wissenschaftspark Potsdam-Golm, D-14424 Potsdam, Germany

The novel beamline P03 (Micro- and Nanofocus X-ray Scattering, MiNaXS) at PETRA III serves a nano- and microfocus end station for performing small- and wide-angle x-ray scattering (SAXS/WAXS) experiments. With its microfocus end station being now in full user operation, its versatility allows for incorporating advanced complementary methods, such as fluidics and imaging ellipsometry [1]. To highlight the unique research capabilities at MiNaXS in terms of microfocused x-ray beams, low divergence and time-resolution, we present the results of in-situ spray and high-rate sputter deposition. The combination of high local and temporal resolution enables the in-situ observation of the fast deposition and nanostructure build-up in combination with microbeam grazing incidence small-angle x-ray scattering (μGISAXS): The nanostructure build-up is locally analyzed from the initial deposition stages to the late vertical nanostructure and domain build-up with ms time resolution.

[1] S.V. Roth et al., J. Phys: Cond. Matter 23, 254208 (2011)

CPP 26.6 Wed 11:00 Poster A

A 2D waveguide beam for X-ray nanodiffraction

— •Christina Krywka[1], Henrike Neubauer[2], Marius Priebe[2], Tim Salditt[2], Jozef Keckes[3], Stjepan Hrkac[1], Adeline Buffet[4], Stephan Roth[4], Ralph Doehrmann[4], and Martin Müller[5] — [1]Christian-Albrechts-Universität zu Kiel, Institut für Experimentelle und Angewandte Physik, Leibnizstr. 19, D-24098 Kiel — [2]Georg-August-Universität Göttingen, Institut für Röntgenphysik, Friedrich-Hund-Platz 1, D-37077 Göttingen — [3]Montanuniversität Leoben, Department Materialphysik, Jahnstr. 12/I, A-8700 Leoben — [4]DESY, Notkestr. 85, D-22603 Hamburg — [5]Helmholtz Zentrum Geesthacht, Max-Planck-Str. 1, D-21502 Geesthacht

The applicability of an X-ray nanobeam generated using a 2-dimensionally confining waveguide is demonstrated for nanodiffraction purposes. The experiments were performed at the Nanofocus extension of MINAXS Beamline at PETRA III. The Nanofocus extension of MINAXS is designed to routinely provide a nanofocused X-ray beam for diffraction experiments and is operated by the University of Kiel. Next to an extensive characterization of the waveguide beam, first high resolution nanodiffraction experiments were performed, e.g. on nanocrystalline TiN hard coatings on WC-Co and on ZnO-microrods with a microscopic metallic coating. Using the high spatial resolution of the waveguide beam interfacial residual stress was revealed in both sample systems. Finally, this contribution presents the current status and future extensions of the Nanofocus endstation.

CPP 26.7 Wed 11:00 Poster A

Easy use and low cost fibre based two color dynamic light scattering — Achim Lederer and ●Hans Joachim Schöpe — Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Deutschland

Light scattering (LS) is one of the most powerful tools in soft matter physics to study the single particle properties as well as the structure, kinetics and dynamics of the system of interest. Unfortunately multiple scattering often complicates the data evaluation. A classy way to circumvent multiple scattering effects in LS data is provided by cross-correlation techniques [1]. Here two identical but distinguishable dynamic light scattering experiments are performed simultaneously on the same scattering volume, which is a major challenge to the mechanical and optical design of the setup. We present a new designed small and compact two color cross correlation light scattering setup to study the structure and dynamics of colloidal suspensions in the regime of considerable turbidity. Using a home-made concentric four arm goniometer, combined with fiber optical illumination and detection devices allows an easy and long time stable alignment - even under temperature variation of ~5°C. Tests with a nearly multiple scattering free suspension of small Rayleigh scatterers show intercepts in cross correlation near 0.4 over a wide range of scattering angles from 20° to 150°. Measuring slightly turbid samples in cross correlation mode multiple scattering is sufficiently suppressed allowing the determination of multiple scattering free dynamic structure factors as well as particle form factors.[1] K. Schätzl, Journal of Modern Optics 38, 1849 (1991)

CPP 26.8 Wed 11:00 Poster A

Conceptual design for a small angle neutron scattering instrument at a long pulse source — ●Damian Martin Rodriguez[1], Henrich Frielinghaus[2], and Dieter Richter[1] — [1]ICS and JCNS, Forschungszentrum Juelich GmbH, 52425 Juelich, Germany — [2]JCNS outstation FRM2, Forschngszentrum Juelich GmbH, Lichtenbergstr. 1, 85747 Garching, Germany

Within the European Spallation Source (ESS) Design Update Programme we are studying several concepts for a time of flight small angle neutron scattering (TOF-SANS) instrument for a long pulse source, i.e. the ESS in Lund. The favourite concept aims at samples of 1 x 1 cm^2 area, which is directly connected with a 10 + 10 m. long SANS instrument or even longer. For a large spanned Q range we propose the use of at least two detectors at different distances. So for one-shot kinetic experiments the classical SANS Q-range can be covered. These initial considerations lead to a simple instrument with little compromises. Extensions for this basic set-up are considered as add-ons, like focussing optics, size changing slits or polarising elements.

The overall design will serve nearly all possible topics for the future research need for the SANS users around Europe.

CPP 27: Poster: (Hydrogels) and Elastomers

Time: Wednesday 11:00–13:00 Location: Poster A

CPP 27.1 Wed 11:00 Poster A

Cononsolvency in aqueous solutions of P(S-*b*-NIPAM) diblock copolymers — ●Konstantinos Kyriakos[1], Martine Philipp[1], Joseph Adelsberger[1], Sebastian Jaksch[1], Anna Miasnikova[2], Andre Laschewsky[2], Isabelle Grillo[3], Peter Müller-Buschbaum[1], and Christine M. Papadakis[1] — [1]TU München, Physik Department, Physik weicher Materie, Garching — [2]Universität Potsdam, Institut für Chemie — [3]ILL, Grenoble

Thermoresponsive hydrogels have attracted a lot of attention as switches. PNIPAM exhibits a lower critical solution temperature (LCST) of 32 °C. Moreover, PNIPAM exhibits the cononsolvency effect, i.e. a miscibility gap upon addition of a second polar solvent, e.g. methanol. Diblock copolymers consisting of a long thermoresponsive PNIPAM block and a short hydrophobic polystyrene block (P(S-*b*-NIPAM)), are of great interest regarding their tendency to form core-shell micelles in aqueous solution.

We report here on a stopped-flow experiment with time-resolved SANS on P(S-*b*-NIPAM) diblock copolymers in micellar solution in D_2O to which d-MeOH was added in various mixing ratios. The focus is on the micellar structure and the correlation between the micelles. For all chosen solvent ratios, the growth of clusters with final sizes between 40 nm and 50 nm is observed.

CPP 27.2 Wed 11:00 Poster A

Rate Theory of Cyclic Structures in Polymer Model Networks — ●Michael Lang[1], Konrad Schwenke[1,2], and Jens-Uwe Sommer[1] — [1]Leibniz Institut für Polymerforschung Dresden e.V., Hohe Straße 6, 01069 Dresden, Germany — [2]Institut f. Baustoffe (IfB), ETH Zürich, Schafmattstrasse 6, 8093 Zürich, Switzerland

A rate theory of the homo- and co-polymerization of f-functional molecules is developed, which contains the formation of short cyclic structures inside the network. The predictions of this model are compared with Monte-Carlo simulations of network formation. We find that homo-polymerizations are well captured by mean-field models at concentrations larger than one quarter of the geometrical overlap concentration. A comparison with the simulation data reveals that correlations among multiply connected molecules can be neglected for these samples. Co-polymerizations are considered in the case of a strict A-B reactions, where all reactive groups of individual molecules are either of type A or type B . For these systems we find a strong influence of density fluctuations of both species for all concentrations investigated. The effect of fluctuations is more than compensated by the lack of ring structures containing an odd number of molecules as compared to homo-polymerizations. Therefore, network formation is readily possible at concentrations one order of magnitude below the overlap concentration. Based on our data we conclude that fluctuation effects are important for co-polymerizations and that mean-field models are less appropriate for their description.

CPP 27.3 Wed 11:00 Poster A

Interaction of Au-NPs with p-NIPAM microgel particles — ●Kornelia Gawlitza[1], Matthias Karg[2], Paul Mulvaney[3], and Regine von Klitzing[1] — [1]Stranski-Laboratorium, Institut für Chemie, Technische Universität Berlin, Germany — [2]Physical Chemistry I, University of Bayreuth, Germany — [3]School of Chemistry & Bio21 Institute, University of Melbourne, Australia

In the last decades, gold nanoparticles (Au-NPs) have been used for the preparation of hybrid materials that combine organic and inorganic components.[1] Due to the thermoresponsibility of poly-N-Isopropylacrylamide (p-NIPAM) microgel particles they are of interest for a lot of applications. In the literature, the usage of Au-NPs to investigate the structure of p-NIPAM microgel particles is discussed.[2] In the present study, Au-NPs with a diameter of 18 nm were synthesized and incorporated within p-NIPAM microgel particles with a varying crosslinker content of 0.25%, 5% and 10%. By using Transmission Electron Microscopy (TEM), cryo-TEM and UV-VIS-spectroscopy, the location of the Au-NPs within the polymer network was determined. As result, the Au-NPs are only located in the outer shell of the polymer network. Additionally, an increase in temperature above the lower critical solution temperature (LCST) leads to a Plasmon-coupling which can be shown by a red shift of the absorption maximum. [1] *R. Contreras-Cáceres, A. Sánchez-Iglesias, M. Karg, I. Pastoriza-Santos, J. Pérez-Juste, J. Pacifico, T. Hellweg, A. Fernández-Barbero, L. M. Liz- Marzán, Adv. Mater. 2008, 20, 1666. [2]*M. Kuang, D. Wang, H. Möhwald, Adv. Funct. Mater. 2005, 15, 1611.

CPP 27.4 Wed 11:00 Poster A

Thermoresponsive microgels prepared using a semi-batch emulsion polymerization — •Sarah T. Turner and Regine von Klitzing — Stranski Laboratory, Dept. of Chemistry, TU Berlin, Germany

The ability to reversibly switch between a collapsed and expanded state in response to an external stimulus, such as temperature or pH-value, makes microgels attractive for applications such as sensoric and drug delivery systems. Thermoresponsive microgels prepared using a batch emulsion polymerization are known to contain inhomogeneities in the crosslinking density distribution due to the variation in the monomer and crosslinker reactivities [1]. A semi-batch emulsion polymerization is a versatile alternative to a batch polymerization for the preparation of microgels that provides a more homogeneous internal crosslinking distribution, compared to the batch emulsion polymerization, when the feed rate is set to the consumption rate of the various monomer components [2]. Here, we present the results of kinetic and morphological studies on microgels prepared by batch and semi-batch methods. Moreover, the preparation and response of hybrid microgels containing metallic nanoparticles implementing the semi-batch method are studied.

[1] X. Wu et al. *Coll. Polym. Sci.* **272**, 467 (1994). [2] R. Acciaro et al. *Langmuir* **27**, 7917 (2011).

CPP 27.5 Wed 11:00 Poster A

Star-PEG-Heparin-Polyelectrolyte-Hydrogels - Network Structure — •Ron Dockhorn[1,2] and Jens-Uwe Sommer[1,2] — [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 hydrogels made of heparin, a rod-like highly charged glycosaminoglycan as a highly functionalized cross-linker, and non-charged, elastic 4-star-shaped-polyethylene glycol. We focus on the network structure by using the bond-fluctuation simulation method and determine the defects, the topological arrangement, and percolation threshold of the gels. Also, we investigate the influence of the initial molar ratio, the variations of functionalized groups, and the concentration dependence of the reaction mixture. We developed a mean-field type model to understand the combined effects of counterions and a good solvent on the swelling properties of the gels [1]. It has been shown that this interplay leads to nearly constant heparin concentration in the swollen gel under physiological conditions, while large variations of the degree of swelling and the storage modulus are accessible. This gels allow a constant release of heparin-binding signaling molecules while independently controlling the mechanical properties to optimize matrices with both mechanical and biomolecular features for cell replacement-based therapies.

[1] Sommer, J.-U., Dockhorn, R. et al., Swelling Equilibrium of a Binary Polymer Gel, Macromolecules 2011 44 (4), 981-986

CPP 27.6 Wed 11:00 Poster A

Structure-Function-Relationships in Biomimetic Hydrogels — •Valentin Hagel, Seraphine Wegner, Yvonne Schoen, Isabell Nuss, Tamas Haraszti, Heike Boehm, and Joachim Spatz — Max Planck Insitute for Intelligent Systems, Department New Materials and Biosystems, Stuttgart, Germany & University of Heidelberg, Department of Biophysical Chemistry, Heidelberg, Germany

Hydrogels are extensively studied as matrices for tissue engineering applications. The importance of these materials comes from their chemical versatility that allows for the design of a broad range of gels with tunable properties and their excellent biocompatibility due to their physical similarity to the native extracellular matrix. Engineering the mechanical and structural properties of hydrogels allows to design feasible materials for tissue repair implants. We present the analysis of hyaluronan-based hydrogels formed with a new type of biomimetic cross-linker. For the characterization of the polymer morphology and transport phenomena within the gels FRAP is used and a diffusion model is derived from the obtained data. Mechanical and rheological analyses are done on a mechanical testing system and a rotational rheometer. The results from both the mechanical and the diffusion analysis are correlated in order to establish structure-function-relationships.

CPP 27.7 Wed 11:00 Poster A

Tracer diffusion in hydrogels — •Peter Kosovan, Olaf Lenz, and Christian Holm — Institute of computational physics, University of Stuttgart, Germany

In this work we consider the diffusion behaviour of a simple spherical tracer particle in polymer networks of hydrogels. There have been hints detained via Fluorescence Correlation Spectroscopy on anomalous diffusion of FCS tracer particles in a hydrogel. We investigate by means of MD simulation the diffusion properties of a tracer particle in the presence of polymer chains with which it interacts. With a sufficiently strong tracer-polymer interaction, subdiffusive behaviour is observed on intermediate time scales and normal diffusive on long time scales. The observation is rationalised via a simple two-state model.

CPP 27.8 Wed 11:00 Poster A

MD simulations of charged hydrogels under external pressure: perspective for seawater desalination — •Tobias Richter, Peter Kosovan, and Christian Holm — Institute of computational physics, University of Stuttgart, Germany

Recent experiments show that application of mechanical pressure on charged hydrogels can be utilised to extract water with a lower salt content than the original solution in which the gel was swollen. It has been suggested to utilise this for an inexpensive method of obtaining desalinated water. We performed a series of MD simulations systematically investigating equilibrium between charged hydrogels under compression and a salt solution. In particular, we investigate the influence of chain length, degree of charging of the hydrogel and concentration of the original salt solution on the salt concentration in the obtained desalinated water.

CPP 27.9 Wed 11:00 Poster A

Microscopic modelling of magneto-sensitive elastomers: lattice approaches — •Dmytro Ivaneyko[1,2], Vladimir Toshchevikov[2], Marina Saphiannikova[2], and Gert Heinrich[1,2] — [1]Institute of Materials Science, Technical University of Dresden, 7 Helmholtz Str., 01069 Dresden, Germany — [2]Leibniz Institute of Polymer Research Dresden, 6 Hohe Str., 01069 Dresden, Germany

We propose a theory which describes the mechanical behaviour of magneto-sensitive elastomers (MSEs) under a uniform external magnetic field. We focus on the MSEs with isotropic spatial distribution of magnetic particles. A mechanical model is used in which magnetic particles are arranged on the sites of three regular lattices: simple cubic, body-centered cubic and hexagonal close-packed lattices. By this we extend our previous approach [1] which used only the simple cubic lattice for describing the isotropic spatial distribution of the particles. The magneto-induced deformation and the Young's modulus of MSEs are calculated as functions of the strength of the external magnetic field. We show that the magneto-mechanical behaviour of MSEs is very sensitive to the spatial distribution of the magnetic particles. MSEs can demonstrate either uniaxial expansion or contraction along the magnetic field and the Young's modulus can be an increasing or decreasing function of the strength of the magnetic field depending on the spatial distribution of the magnetic particles.

[1] Ivaneyko, D.; Toshchevikov, V.P.; Saphiannikova, M.; Heinrich, G., Macromolecular Theory & Simulations 2011, 20, 411-424

CPP 27.10 Wed 11:00 Poster A

Switching Behavior of Thermoresponsive Poly(2-oxazoline) Copolymers — •Sebastian Jaksch[1], Stephan Salzinger[2], Stephan Huber[2], Joseph Adelsberger[1], Peter Busch[3], Rainer Jordan[4], and Christine M. Papadakis[1] — [1]TU München, Physikdepartment, Physik der weichen Materie, Garching — [2]TU München, Department Chemie, Lehrstuhl für Makromolekulare Chemie, Garching — [3]JCNS-FRM II, Garching — [4]TU Dresden, Department Chemie, Professur für Makromolekulare Chemie, Dresden

Thermoresponsive polymers in aqueous solution exhibit a strong change in solubility and volume when heated above their cloud point. Especially interesting polymers of this class of materials are poly(2-oxazoline)s (POx) which are biocompatible. We investigate poly[(*iso*-propyl-2-oxazoline)-*grad*-(*n*-nonyl-2-oxazoline)] gradient copolymers where the fraction of the hydrophic nonyl moieties is varied. These moieties are found to lower the cloud point from 41°C to 23°C. In order to elucidate the aggregation behavior around the cloud point we performed small-angle neutron scattering experiments. The unimer radii increase upon heating towards the cloud point which is consistent with an onset of aggregation. Above the cloud point, we first encounter an intermediate regime, where, instead of the expected collapse, the small aggregates formed below the cloud point, dominate. Large aggregates are only formed a few Kelvin above the cloud point.

[1] S. Salzinger, S. Jaksch, C.M. Papadakis et al., Coll. Polym. Sci. accepted

CPP 27.11 Wed 11:00 Poster A

Swelling and switching behavior of thermo-responsive P(S-b-MDEGA-b-S) hydrogel films under vapor atmosphere — •Qi Zhong[1], Ezzeldin Metwalli[1], Monika Rawolle[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, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]Potsdam Universität, Inst. Chemie, Karl-Liebknecht-Str. 24-25, 14476 Potsdam-Golm, Germany — [3]ILL, 6 rue Jules Horowitz, 38000 Grenoble, France

By a change of temperature below or above the lower critical solution temperature (LCST), thermo-responsive hydrogels switch between a swollen and a collapsed state. The thermo-responsive poly(monomethoxy diethyleneglycol acrylate) (PMDEGA) exhibits a higher LCST (39.6 oC) as compared to the frequently investigated poly(N-isopropylacrylamide) (PNIPAM), which can be advantageous for many applications. To introduce an internal ordering, a tri-block copolymer with hydrophobic polystyrene end-blocks is under investigation. P(S-b-MDEGA-b-S) films are successfully prepared by spin-coating. The response of P(S-b-MDEGA-b-S) films to a sudden thermal stimulus is probed. To study this switching behaviour, in-situ neutron reflectivity is used. P(S-b-MDEGA-b-S) films subjected to different thermal stimuli are under investigation.

CPP 27.12 Wed 11:00 Poster A

Elastic anomalies at the volume phase transition of PNIPAM solutions — •Martine Philipp[1], Ulrich Müller[2], Olga Astasheva[2], Jan Krüger[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, Garching, Germany — [2]Université du Luxembourg, Laboratoire de physique des matériaux avancés, Luxembourg, Luxembourg

The molecular collapse of poly(N-isopropyl acrylamide) (PNIPAM) in aqueous solution at the lower critical solution temperature has been intensively investigated in basic and applied research. On a macroscopic scale, this phase transition is reflected in an anomalous behavior of the mass density and elastic properties. Particularly in case of chemical PNIPAM hydrogels, the longitudinal elastic modulus is considered as the order parameter susceptibility of the highly complex volume transition. In the current contribution the evolution of elastic anomalies at the discontinuous volume transition of PNIPAM solutions is presented in dependence of temperature and PNIPAM concentration. Brillouin spectroscopy permits a novel and unique perspective on the static, dynamic and kinetic aspects of the phase separation occurring at about 32°C. In particular the qualitative changes of the acoustic phonon spectrum at the phase transition reflect the formation of macroscopic PNIPAM-rich agglomerates embedded in the PNIPAM-poor phase.

CPP 27.13 Wed 11:00 Poster A

On the structure of Star Polymer Networks — •Michael Lang[1], Konrad Schwenke[1,2], and Jens-Uwe Sommer[1] — [1]Leibniz Institut für Polymerforschung Dresden e.V., Hohe Straße 6, 01069 Dresden, Germany — [2]Institut f. Baustoffe (IfB), ETH Zürich, Schafmattstrasse 6, 8093 Zürich, Switzerland

Using the bond fluctuation model we study polymer networks obtained by end-linking of symmetric 4-arm star polymers. We consider two types of systems. Solutions of one type (A) of star polymers and solutions of two types (A,B) of star polymers where A-type polymers can only crosslink with B-type polymers. We find [1] that network defects in A networks are dominated by short dangling loops close to overlap concentration c^*. AB networks develop a more perfect network structure, since loop sizes involving an odd number of stars are impossible, and thus, the most frequent dangling loop with largest impact on the phantom modulus is absent. The analysis of the pair-correlation and scattering function reveals an amorphous packing of A and B type stars in contrast to the previously suggested crystalline like order of A and B components at c^*. Furthermore, we derive the vector order parameters associated with the most frequent network structures based on the phantom model. In particular for AB networks we can show that there is a dominating cyclic defect with a clearly separated order parameter that could be used to analyze cyclic network defects.

[1] K. Schwenke, M. Lang, J.-U. Sommer, Macromolecules, *in press.*

CPP 27.14 Wed 11:00 Poster A

Static, dynamic and kinetic property changes around the collapse transition of PNIPAM solutions as seen by Temperature Modulated Optical Refractometry — •Ralitsa Aleksandrova[1], Ulrich Müller[1], Martine Philipp[1,2], Roland Sanctuary[1], Peter Müller-Buschbaum[2], and Jan-Kristian Krüger[1] — [1]Université du Luxembourg, Faculté des Sciences, de la Technologie et de la Communication 162 A, avenue de la Faïencerie L-1511 Luxembourg — [2]Technische Universität München, Physik-Department E13, Lehrstuhl für Funktionelle Materialien, 85747 Garching, Germany

The collapse transitions of aqueous PNIPAM solutions are investigated by the novel technique of Temperature Modulated Optical Refractometry (TMOR) as a function of temperature and time. In addition to the refractive index, TMOR yields information about the real and imaginary part of the thermo-optical coefficient and the volume coefficient of thermal expansion. Since all these physical quantities couple rather directly to the order parameter of the collapse or volume phase transition, they are able to shed new light on the structure formation during the collapse phase of aqueous PNIPAM solutions on a mesoscopic and macroscopic scale.

CPP 27.15 Wed 11:00 Poster A

Visualization of the Coil-Globule Transition of a Thermoresponsive Polymer in Mixtures with a Conjugated Polyelectrolyte — •Sahika Inal[1], Jonas D. Kölsch[2], Dietmar Janietz[3], André Laschewsky[2], Ullrich Scherf[4], and Dieter Neher[1] — [1]Inst. of Physics and Astronomy, Uni. of Potsdam, Germany — [2]Department of Chemistry, Uni. of Potsdam, Germany — [3]Fraunhofer Inst. for Applied Polymer Research, Germany — [4]Macromolecular Chemistry Group, Bergische Uni. Wuppertal, Germany

Changes in the physical environment of smart polymers alter the intermolecular interactions that stabilize their chains in water, which translates into macroscopic responses such as coil to globule transition. Here, we present a scheme to optically visualize the temperature-induced coil to globule transition of a smart polymer using Förster resonance energy transfer (FRET). The aqueous mixtures of a cationic conjugated polymer electrolyte and a dye-labeled nonionic thermoresponsive polymer at room temperature exhibit reduced fluorescence intensity from the responsive polymer, accompanied by an enhanced emission from the polyelectrolyte, indicative of FRET mechanism. Heating this mixture above the cloud point of the smart polymer strongly reduces the efficiency of FRET. We propose that the two macromolecules form mixed aggregates at room temperature, and that these aggregates are disrupted upon the coil-globule transition. As a consequence, temperature-induced structural changes in these macromolecular complexes are detected as well visible variations of fluorescence signal. This visualization scheme shall be well applicable to biochemical sensors.

CPP 27.16 Wed 11:00 Poster A

Phase-transition actuator — •Roland Altmueller, Reinhard Schwoediauer, Siegfried Bauer, and Ingrid Graz — Soft Matter Physics, Institute for Experimental Physics, J. Kepler University, Altenbergerstrasse 69, 4040 Linz, Austria

Dielectric elastomers have widespread applications in sensing, for energy harvesting and actuation. By applying a sufficiently large voltage the elastomer in between two compliant electrodes deforms and complex shapes such as grippers or walkers are realized. However, the required driving voltages are large, often in the kilovolt range, so the reduction of the driving voltage has been identified as a key challenge in the field.

Here we present phase-transition actuators where an elastomeric frame undergoes large deformations caused by the phase transition of an embedded liquid from the liquid to the gaseous state. The phase transition in the liquid is simply induced by electrical Joule heating. A very large deformation is feasible on the base of the huge volume changes upon the liquid gaseous phase transition. Low voltage operation is guaranteed, since the deformation relies on liquid heating, albeit with larger power consumption in comparison to DEAs.

Biaxial deformations of up to 120 % are achieved in a 9 mm wide liquid reservoir within a PDMS elastomer at a driving voltage of 10 V and an input power of 1 W, with a large blocking force of 5-6 N. The proposed actuator concept is easily prone to miniaturization, potentially useful in Braille readers.

CPP 27.17 Wed 11:00 Poster A

Local stress distributions in strained elastomers by low-field NMR — •Maria Ott[1], Martin Schiewek[1], Horst Schneider[1], Paul Sotta[2], and Kay Saalwächter[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Faculty of Natural Science II, Betty Heimann Str 7, 06120 Halle, Germany — [2]Laboratoire de physique des solides, Université Paris-Sud, Bât. 510, 91405 Orsay Cedex, France

Macroscopic strain applied to elastomeric networks induces reorientations of the constituent polymer chains. In this way, heterogeneities of the polymer matrix become apparent, reflecting a potentially nontrivial and complex distribution of local stresses, which is particulary relevant for elastomers with nanofillers. We present a general NMR approach [1] which enables to study the molecular-level effect of macroscopic strain by revealing the absolute values and the distributions of the average segmental residual dipolar couplings. These reflect the time-averaged orientation of the polymer backbone and are directly related to the local stress [2]. We demonstrate this approach using natural rubber of different cross-link densities and amounts of filler particles. We found new fractions of highly coupled (stressed) chain segments which increase with the applied strain. However, a large discrepancy of the overall increase reveals the limits of the well-established Gaussian model [3], and a new theoretical approach is discussed.

[1] K. Saalwächter, Prog. Nucl. Magn. Reson. 51, 1-35 (2007)
[2] J.-U. Sommer et al., Phys. Rev. E 78, 051803 (2008)
[3] P. Sotta, B. Deloche, Macromolecules 23, 1999-2007 (1990)

CPP 28: Colloids and Complex Liquids I

Time: Wednesday 15:00–18:45 Location: C 130

Invited Talk CPP 28.1 Wed 15:00 C 130

The glass transition is continuous but gelation is discontinuous in sticky spheres — •Paddy Royall[1], Stephen Williams[2], and Hajime Tanaka[3] — [1]University of Bristol, UK — [2]Australian National University, Canberra, Australia — [3]The University of Tokyo, Japan

We identify dynamic and structural signatures which distinguish gels and glasses in a colloidal model system of hard and sticky spheres. Since gels are identified with arrested spinodal decomposition, this presents a thermodynamic basis upon which to identify gelation, and distinguish it from vitrification. We base our findings on confocal microscopy experiments of and confirm these with molecular dynamics simulations.

In the gel transition, upon crossing the spinodal line at a packing fraction 0.35, we find a sharp change in the structural relaxation time, and enter an ageing regime. Simultaneously, our novel structural analysis shows a large and sudden change in local structure. This is confirmed in simulation where the pressure turns negative upon gelation. Thus gelation is 'first-order-like'. By contrast, the approach to the glass is continuous, and not associated with any phase transition.

In 'sticky spheres', since gelation occurs at the spinodal line, it appears 'first-order-like', while on the timescales we access, the glass transition is continuous. Arrested states lying in the metastable gas-liquid regime are gels and those outside glasses. Significantly, the gel extends to packing fractions of at least 0.59.

CPP 28.2 Wed 15:30 C 130

Zigzag transition and nonequilibrium explosions in a one-dimensional colloidal crystal — •Arthur Straube[1], Lutz Schimansky-Geier[1], Roel Dullens[2], and Ard Louis[3] — [1]Department of Physics, Humboldt University of Berlin, Germany — [2]Physical and Theoretical Chemistry Laboratory, Department of Chemistry, University of Oxford, UK — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, UK

We study the equilibrium zigzag transition and nonequilibrium pattern formation that emerges when magnetically repelling colloids, trapped individually in a line by optical tweezers, are abruptly released, forming colloidal explosions [EPL **94**, 48008 (2011); J. Chem. Phys., submitted]. We show experimentally and explain theoretically why for certain nonharmonic traps the equilibrium zigzag transition is impossible. Colloidal explosions demonstrate a nonequilibrium zigzag pattern that persists even when magnetic interactions are much weaker than those that break the linear symmetry in equilibrium. Theory and computer simulations, including hydrodynamic interactions, quantitatively describe these phenomena both in and out of equilibrium.

CPP 28.3 Wed 15:45 C 130

Wrinkle-assisted linear assembly of plasmonic-core/soft-shell particles: A lithography-free approach towards anisotropic nanostructures — •Mareen Mueller[1], Matthias Karg[2], Andrea Fortini[3], Thomas Hellweg[4], and Andreas Fery[1] — [1]Physical Chemistry II, University of Bayreuth, Germany — [2]Physical Chemistry I, University of Bayreuth, Germany — [3]Theoretical Physics II, University of Bayreuth, Germany — [4]Physical Chemistry III, University of Bielefeld, Germany

This contribution addresses wrinkle assisted assembly of silver-poly-(N-isopropylacrylamide) core-shell particles. Anisotropic alignment is found on two length scales, macroscopically guided through the wrinkle structure and locally due to deformation of the polymer shell leading to smaller inter-core separations as compared to assembly on flat substrates without confinement. The structures were analyzed by means of scanning electron microscopy. Radial distribution functions are shown, clearly highlighting the impact of confinement on nearest neighbor distances and symmetry. The observed ordering is directly compared to Monte-Carlo simulations for hard-core/soft-shell particles, showing that the observed symmetries are a consequence of the soft interaction potential and differ qualitatively from a hard-sphere situation. As a first evidence for the impact of the alignment on optical properties, we show UV-vis absorbance measurements revealing optical anisotropy of the generated structures due to plasmon coupling. Furthermore, the high degree of order of the assembled structures on macroscopic areas is demonstrated by laser diffraction effects.

CPP 28.4 Wed 16:00 C 130

Guided self-assembly of microgels: From particle arrays to anisotropic nanostructures — •Marco-Philipp Schürings[1], Patrick Wünnemann[1], Stephanie Hiltl[1], Andrij Pich[2], and Alexander Böker[1] — [1]Lehrstuhl für Makromolekulare Materialien und Oberflächen RWTH Aachen, D-52056 Aachen, Germany — [2]Lehrstuhl für Funktionale und Interaktive Polymere, RWTH Aachen, D-52056 Aachen, Germany

Our work aims at the production of microgel strings, rods and meshes via crosslinking of well-defined particle arrays. Wrinkled substrates are prepared by oxidization of stretched Polydimethylsiloxane (PDMS). Subsequently, microgels of N-vinyl caprolactam/Acetoacetoxy ethylmethacrylate (VCL/AAEM) and N-isopropylacrylamide/N-vinylcaprolactam (NIPAAm/VCL) are spin-coated onto these surfaces thereby forming self-assembled structures within the wrinkle grooves. We consequently transfer those pre-aligned particles onto flat silicon wafers to create periodic nanostructures covering large surface areas up to 3 x 3 cm, as confirmed by GISAXS measurements. UV irradiation of the assembled particles yields microgel chains with variable widths of 500- 2000 nm and lengths up to 27 microns which are tunable by altering the wavelength of the PDMS wrinkles. Due to the thermoresponsiveness of VCL/AAEM colloids anisotropic contraction can be induced, which leads to possible applications as sensors and actuators. By using light or electrosensitive microgels and considering their biocompatibility even more applications, such as synthetic muscle fibers, appear feasible.

CPP 28.5 Wed 16:15 C 130

Core size effects on the rotation and stability of dipolar clusters in rotating magnetic field — •Ayan Ray and Thomas M. Fischer — Institut für Experimentalphysik, Universität Bayreuth, 95440 Bayreuth, Germany.

We report on the rotation of colloidal clusters of non magnetic holes and of mixtures of paramagnetic beads with non magnetic holes in a ferrofluid in a rotating external magnetic field. The precession angle of the external field is a control parameter determining the stability of the cluster. Clusters become locally unstable when the local precession angle reaches the magic angle. Cluster shape dependant depolarization fields lead to a deviation of the local from the external precession angle such that close to the external magic angle different cluster shapes might coexist. For this reason cluster transitions are weakly or strongly first order transitions. If the transition is weakly first order a critical speeding up of the cluster rotation is observed. No speeding up occurs for strongly first order cluster transitions with hysteresis. The strength of the first order transition is controlled by the size of the core of the cluster.

CPP 28.6 Wed 16:30 C 130

Well-defined colloidal clusters by combined chemical and topographical templating — •Christoph Hanske[1], Alexander Wittemann[2], and Andreas Fery[1] — [1]Physical Chemistry II, University of Bayreuth, Germany — [2]Physical Chemistry I, University of Bayreuth, Germany

Assemblies of colloidal particles are promising building blocks for future lab-on-a-chip devices such as sensors. Recently, we have introduced the creation of large-scale ordered arrays of particles using wrinkled elastomers (1, 2). These wrinkled stamps are accessible by the systematic exploitation of buckling instabilities without any lithographic steps. By placing a wrinkled stamp onto a droplet of colloidal suspension, liquid filled channels are formed confining the particles. Due to capillary forces close packed arrays are formed during drying. While the procedure is applicable to a wide range of particles, successful colloidal assembly strongly depends on interfacial properties. In this contribution we concentrate on the influence of the wettability of both the stamps and the substrates on the deposition process. Furthermore, local variations of the wettability can be achieved by microcontact printing. Combing such chemically patterned substrates with topographical templating in wrinkles allows us to create colloidal clusters in highly regular arrangements.

1. Lu, C.; Möhwald, H.; Fery, A. Soft Matter 2007, 3, 1530-1536.
2. Schweikart, A.; Fortini, A.; Wittemann, A.; Schmidt, M.; Fery, A. Soft Matter 2010, 6 (23), 5860-5863.

15 min break

CPP 28.7 Wed 17:00 C 130

Smart Microgel Capsules and Model Colloids Tailored by Droplet-Based Microfluidics — •Sebastian Seiffert — Helmholtz Zentrum Berlin, F-I2 Soft Matter and Functional Materials, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Micrometer-sized polymer gel particles can be produced with exquisite control by droplet-based microfluidics. The idea of this approach is to use emulsion droplets as templates to control the particle size, shape, and monodispersity. To extend this control towards controlling the material properties of the microgels, microfluidic templating can be combined with the use of functional, macromolecular precursors; this separates the polymer synthesis from the particle gelation and allows each to be controlled independently. It also allows complex morphologies such as hollow, anisotropic, or multi-layered microgels to be formed and complexed with additives such as drugs, colloids, or living cells. In addition to their utility for encapsulation, these microgels can serve as model systems to explore how the particle stiffness and size affect the bulk and shear elasticity of compressed particulate suspensions. While it is known that in dilute solution, the dynamics of colloidal microgels strongly dependends on the particle size, it is unclear to what extent the dynamics of microgel systems is determined by the particle size if the system is densely packed. A droplet-based microfluidic approach allows such dense-packed microgel systems to be prepared with particles of strongly varying size, revealing that the isotropic compressibility and shear elasticity of both colloidal-scale and granular-scale systems show universal, macrogel-type scaling independent of the particle size.

CPP 28.8 Wed 17:15 C 130

How Hidden Degrees of Freedom affect Fluctuation-Theorems — •Jakob Mehl[1], Boris Lander[2], Udo Seifert[2], Clemens Bechinger[1], and Valentin Blickle[1] — [1]2. Physikalisches Institut, Universität Stuttgart, Germany — [2]II. Institut für Theoretische Physik, Universität Stuttgart, Germany

Fluctuation-theorems (FT) are one of the few exact relations, which are valid for systems driven out of equilibrium. The connection between the free energy difference and the work done to a system, known as Jarzynski equality, is certainly the most prominent example of the FT for the total entropy production Δs_{tot}. So far, experimental studies concentrated only on simple systems with one degree of freedom.

By combining paramagnetic colloidal particles and rotating laser tweezers, we study two nonequilibrium steady states, which can be coupled by an externally controlled magnetic field. Using video microscopy, we can simultaneously follow both particles' nonequilibrium fluctuations with high accuracy. As derived from stochastic thermodynamics, all degrees of freedom have to be taken into account to maintain the FT of Δs_{tot}. It is unknown whether such relations change, when only parts of the system are accessible, i.e. when in our experiment only the fluctuations of one particle are regarded. We show that for the prevailing majority of experimental cases the FT is only violated slightly, i.e. only linear correction terms contribute. For extreme situations, strong deviations are present and higher order terms are not longer negligible.

CPP 28.9 Wed 17:30 C 130

Active Brownian Motion in Complex Environments — •Ivo Buttinoni — Universität Stuttgart, Stuttgart, Germany

Active Brownian particles are capable of taking up energy from their environment and converting it into directed motion; examples range from chemotactic cells and bacteria to artificial microswimmers. We develop a novel species of microswimmers whose active motion is due to the local demixing of a critical binary liquid mixture and can be easily tuned by illumination. Illumination causes a local heating of the caps, which induces a local asymmetric demixing of the binary mixture leading to a spatial concentration gradient across the particle. Since the heating strength is controlled by the incident light intensity, the particle's self-diffusiophoretic motion can be easily controlled. As a first step towards more realistic conditions under which such microswimmers will be employed, we study, experimentally and with numerical simulations, their behavior in patterned surroundings that present complex spatial features where frequent encounters with obstacles become important[1]. The motion of such swimmers inside mobile obstacles, i.e., passive colloids, is probed as well, showing memory effects related to the characteristics of both the passive and the active particles.

[1] G. Volpe, I. Buttinoni, D. Vogt, H.J. Kümmerer, and C. Bechinger. Microswimmers in patterned environments. Soft Matter, (7):8810{8815, 2011.

CPP 28.10 Wed 17:45 C 130

DYNAMICAL SIGNATURE OF CRITICALITY IN COLLOIDAL HARD SPHERE LIKE FLUIDS — Markus Franke and •Hans Joachim Schöpe — Johannes Gutenberg Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Germany

The particle dynamics of a metastable liquid differs significantly from a liquid in the equilibrium state, giving the possibility to define the freezing point of the system of interest. Dynamic light scattering gives access to the intermediate scattering function (ISF) which measures particle number density fluctuations. Another aspect of the dynamics is the correlation of particle currents dictated by conservation of particle number density, which can be obtained by numerically differentiating the ISF. Recently it was shown that it is possible to define a dynamic freezing criterion in colloidal hard sphere systems by a careful analysis of the space time correlation function of longitudinal particle currents (CCF) [1]. We used highly cross-linked polystyrene (PS) microgel colloids dispersed in a good solvent to obtain a colloidal model system with hard sphere like interaction. We studied the dynamics of the colloidal fluid around the main structure factor peak (1.7<qR<5) over a wide concentration range crossing the freezing transition. Like in a PMMA hard sphere system we observe an universal scaling of the CCF for the equilibrium fluid, while deviations from this scaling were found once the suspension is in the metastable state. Furthermore it is observed that the decorrelation of the CCF becomes nonmonotonic at the structure factor peak if the fluid becomes overcritical. [1] W. van Megen, V. A. Martinez, and G. Bryant, PRL 103, 258302 (2009)

CPP 28.11 Wed 18:00 C 130

A Poisson-Boltzmann solution of the two-colloid problem — •Alexander Schlaich, Stefan Kesselheim, Marcello Sega, and Christian Holm — Institut für Computerphysik, Universität Stuttgart, Pfaffenwaldring 27, 70569, Stuttgart, Deutschland

The force acting between colloidal particles in ionic solutions is often modeled in terms of the nonlinear Poisson-Boltzmann equation. A solution can be obtained using standard finite element methods, however usual assumptions, like a constant surface charge density at the particle's surface or a constant surface potential, are not able to reproduce the correct potential if the typical distance becomes small such that the Debye layers overlap.

To determine these boundary conditions, we use an iterative procedure which also accounts for a jump of the dielectric constant at the particles surface. We compare our results to theoretical predictions and the results of coarse-grained molecular dynamics simulations using explicit ions. The efficient parallel implementation, using the Distributed and Unified Numerics Environment DUNE, also allows us to consider the question of pairwise additivity in the Poisson-Boltzmann description.

CPP 28.12 Wed 18:15 C 130

Free-standing Fluid Filaments Using Star-shaped and Discotic Liquid Crystal Mesogens — •Tanya Ostapenko, Michael Morys, Alexey Eremin, and Ralf Stannarius — Otto-von-Guericke-Universität, Universitätsplatz 2, 39106 Magdeburg, Germany

Stable free-standing filaments have been formed in several mesophases of bent-core liquid crystals. Such filaments can have slenderness ratios of 1000 or more. In contrast, filaments prepared from columnar liquid crystal phases of disk-shaped molecules have slenderness ratios several orders of magnitude lower, due to the two-dimensional compressibility of the phase. From atomic force microscopy measurements, smectic filaments appear to have a corrugated structure, with composite bundles constructing the filament [1].

Recently, star-shaped oligobenzoates were synthesized [2], which form various liquid crystal columnar mesophases over a large temperature range. To date, there have been no reports on free-standing filaments prepared from such mesophases. Using a similar experimental setup to that described in [1], along with polarizing microscopy, we were able to create meta-stable filaments. We measure optical, mechanical and electrical properties of these unique systems and discuss potential applications.

[1] A. Nemes, et. al. *Phys. Chem. Chem. Phys.* **8**, 469-476 (2005).
[2] M. Lehmann, et. al. *Chem. Eur. J.* **14**, 3562-3576 (2008).

CPP 28.13 Wed 18:30 C 130

Small Angle Scattering applied to Phospholipid stabilized Colloidal Crystals — •Martin Schmiele, Mirijam Zobel, and Tobias Unruh — Lehrstuhl für Kristallographie und Strukturphysik, Staudtstraße 3, D-91058 Erlangen

Many routines do exist to simulate small angle scattering of dispersions of homogeneous nanoparticles, they all rely on the calculation of the particle form factor. However, dispersions of nanocrystals with long crystallographic c-axes may show Bragg peaks in the small angle range. With the existing routines, Bragg reflections can only be taken into account by heuristic models for the peak profiles. In order to compute small angle diffractograms from colloidal dispersions of nanocrystals the X-Ray Powder Pattern Simulation Analysis (XPPSA) has been developed. The XPPSA facilitates the computation of this scattering contribution directly from the crystals geometry. Application-related our group focuses on dispersions of tripalmitin nanocrystals stabilized with phospholipids in an aqueous dispersion medium. They can be considered as a representative model for many similar colloidal dispersions that are currently under discussion as potential drug delivery carrier systems. Revealing the molecular arrangement of the phospholipids at the interface between tripalmitin and the aqueous phase is vitally important to comprehend the stabilization mechanism and to control drug encapsulation. A preliminary study with the aid of the XPPSA utilizing SAXS gave no clear picture for the structure of the stabilizer layer. To remove this ambiguity, SANS experiments at different contrasts for the stabilizer layer were carried out.

CPP 29: Crystallisation, Nucleation and Self assembly

Time: Wednesday 15:00–18:45 Location: C 243

Topical Talk CPP 29.1 Wed 15:00 C 243

Observation of kinks and antikinks in colloidal monolayers driven across ordered surfaces — •Thomas Bohlein[1,2], Jules Mikhael[1], and Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universität Stuttgart, Germany — [2]Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany

Friction between solids is responsible for many phenomena like earthquakes, wear or crack propagation. Unlike macroscopic objects which only touch locally due to their surface roughness, spatially extended contacts form between atomically flat surfaces. They are described by the Frenkel-Kontorova (FK) model which considers a monolayer of interacting particles on a periodic substrate potential. In addition to the well-known stick-slip motion such models also predict the formation of kinks and antikinks which largely reduce the friction between the monolayer and the substrate. Here, we report the direct observation of kinks and antikinks in a two-dimensional colloidal crystal which is driven across different types of ordered substrates. We show that the frictional properties only depend on the number and density of such excitations which propagate through the monolayer along the direction of the applied force. In addition, we also observe kinks on quasicrystalline surfaces which demonstrates that they are not limited to periodic substrates but occur under more general conditions.

Topical Talk CPP 29.2 Wed 15:30 C 243

2D and 3D assembly of polymer-coated gold nanoparticles — •Matthias Karg — Department of Chemistry, University of Bayreuth, Bayreuth, Germany

The assembly of metal nanoparticles into superstructures with mm or even cm dimensions is a challenging scientific task.

We coated gold nanoparticles with cross-linked polymer shells resulting in core-shell particles with well-defined structures[1]. The polymer shells are composed of poly-N-isopropylacrylamide (PNIPAM), which is a thermoresponsive material. Due to these shells, the effective particle volume of the nanoparticles is increased significantly. This allows reaching high volume fractions with comparably low particle numbers.

Crystallization was observed over a broad range of particle concentrations at room temperature[2]. Upon an increase in temperature, the PNIPAM shells shrink and the overall particle volume fraction decreases. This causes melting of the crystals in a certain concentration range. Upon cooling, crystallization occurs again, once a critical volume fraction is reached. These melting/recrystallization processes were observed to occur with very high reproducibility as will be demonstrated in this contribution. This unique behaviour is interesting for applications in sensing and optics since it presents a new pathway towards the controlled preparation of large-scale 'nanocrystal-doped' photonic crystals.

[1] M. Karg, S. Jaber, T. Hellweg, P. Mulvaney, Langmuir 2011, 27, 820 [2] M. Karg, T. Hellweg, P. Mulvaney, Adv. Funct. Mater. DOI: 10.1002/adfm.201101115

CPP 29.3 Wed 16:00 C 243

Lattice orientation, defects, and optical diffraction of opal-type photonic crystals — •Mulda Muldarisnur, Parvin Sharifi, and Frank Marlow — Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr, Germany

A systematic investigation on SEM images reveals that the capillary deposition method (CDM) [1] results in opal films with specific orientations which are interesting photonic crystals [2]. The orientation of the (111) fcc plane parallel to substrate is typical for many opals. However, opal orientation in respect to the growth direction is specific for a certain class of growth methods and indicates a decisive influence of the suspension flow during opal formation. The nearly perfect surface and the oriented lattice allows the existence of two crystal parts (intergrowths) having a certain misfit. The lattice misfit induces disordered boundaries and defects. We found that scattering by these and other defects can be described using Mie-like scattering. Recent angle-resolved transmission measurements and microscopic observations support the existence of two fcc domains in CDM-made opals. We observe well-resolved high-order diffraction peaks indicating opals with high quality. We can very well describe the rich features in the angle-resolved spectra by using the kinematical diffraction theory. Furthermore, intensity variation with angle can be described by using a simplified dynamical diffraction theory.

References: [1] H.-L. Li, W. Dong, H.J. Bongard, F. Marlow, J. Phys. Chem. B 109, 9939 (2005). [2] M. Muldarisnur and F. Marlow, J. Phys. Chem. C 115, 414 (2011).

CPP 29.4 Wed 16:15 C 243

Simulations of colliodial rods on a 2D quasicrystalline substrate — •Philipp Kählitz and Holger Stark — Institut für theoretische Physik, TU Berlin

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 tostudy the phase behavior of micron-sized colloidal particles in a 2D quasicrystalline potential and new ordered phases have been identified [1,2]. This talk discusses how colloidal rods order in a quasicrystalline decagonal substrate potential. We use Monte-Carlo simulations tostudy the phase behavior of hard spherocylinders and identify, in particular, a novel decagonal phase made by clusters of aligned rods at high densities. In the low density case the behavior of the rods is similar to the previously studied hard needles [3]. We map out phase diagrams as a function of strength of the surface potential and the particle density for different rod lengths and diameters.

[1] Mikhael et al., Nature (London) 454, 501 (2008)
[2] M. Schmiedeberg and H. Stark, PRL 101, 218302 (2008)
[3] P. Kählitz and H. Stark, submitted.

CPP 29.5 Wed 16:30 C 243

Homogeneous and flat wall heterogeneous nucleation in colloids with various interaction — Andreas Engelbrecht, Markus Franke, Achim Lederer, Sara Iacopini, Richard Beyer Beyer, and •Hans Joachim Schöpe — Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Deutschland

Understanding crystal nucleation and growth is of great interest in condensed matter physics and material science. Especially at low metastabilities crystal nucleation is dominated by heterogeneous nucleation on container walls or impurities and the competition between wall and bulk crystallization determines the microstructure of the polycrstal. Notwithstanding its relevance heterogeneous nucleation is not well understood. One promising approach to the problem is offered by the study of colloidal suspensions. In colloids the particle interactions can be experimentally adjusted to include short (hard spheres, HS) and long ranged (charged spheres, CS) repulsions as well as attractions originated by entropic forces (attractive spheres, AS). We studied the kinetics of homogeneous and wall induced heterogeneous nucleation in different colloidal model systems with various interaction (CS, HS, AS) as function of super saturation. Using light scattering as well as microscopy techniques a comprehensive analysis of the crystallization process was obtained. We can show that the competition of wall and bulk crystallization is altered significantly with the nature of the particle interaction.

15 min break

CPP 29.6 Wed 17:00 C 243

Self-assembly of amphiphilic Janus particles — •Gerald Rosenthal and Sabine H. L. Klapp — TU Berlin, Institut für Theoretische Physik, Hardenbergstr. 36 , D-10623 BERLIN, Germany

We apply molecular dynamics simulations (MDS) to investigate the structure formation of amphiphilic Janus particles in the volume phase. The Janus particles are modeled as (soft) spheres composed of a hydrophilic and hydrophobic part. Their orientation is described as a vector representing an internal degree of freedom. This model was first proposed by Somoza et al. [1]. In our study we focus on pair correlation functions, cluster characterisation and mean square displacement. We find clusters of various sizes depending on density and temperature. The cluster size distribution shows a narrower peak for higher densities at clusters of size 13, in these icosahedra particles are aligned in closed packing and therefore the number of bondings is maximised. For lower densities a variety of smaller clusters coexists. Further we calculated the aggregation temperature as function of density. In addition to this unconfined system we will compare our newest MDS results in confined geometry with our former classical density functional theory study [2], where we focused on the surface-induced ordering phenomena of such Janus particles.

[1] A. M. Somoza, E. Chacón, L. Mederos and P. Tarazona, J. Phys.: Condens. Matter **7**, 5753 (1995)
[2] G. Rosenthal and S. H. L. Klapp, JCP, **134**, 154707 (2011)

CPP 29.7 Wed 17:15 C 243

Disentanglement during the crystallization of polymers — •Chuanfu Luo and Jens-Uwe Sommer — Leibniz Institute of Polymer Research Dresden, Hohe Str. 6, 01069 Dresden

Long linear polymers are highly entangled in melts while they are folded and packed in crystals. Thus polymer crystallization can lead to some degree of disentanglement of the resulting semi-crystalline material. However this disentanglement process is very difficult to observe in experiments. By using molecular dynamics (MD) simulations combined with primitive path analysis (PPA)[1], we can directly reveal the structural changes of polymer chains as well as the changes of entanglement during the crystallization. The PPA can give the approximated entanglement length from the topology of an instantaneous conformation without running a long-time rheology simulation. By using PPA we analyzed the simulation results of slowly continuous cooling, annealing and self-seeding processes[2]. We show that polymers disentangle during crystallization and continue to disentangle during annealing. The changes of approximated entanglement density at different regions (crystallized Vs. melt) will also be discussed.

[1] R. Everaers et al., Science 303, 823 (2004)
[2] C.-F. Luo and J.-U. Sommer, Macromolecules 44, 1523 (2011)

CPP 29.8 Wed 17:30 C 243

Influence of electric fields on the self assembly of block copolymers in confined geometries. — •Ulrich Welling[1], Hagai Shalev[2], Yoav Tsori[2], and Marcus Müller[1] — [1]Institut für theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Department of Chemical Engineering, Ben Gurion University of the Negev, Beer-Sheva, 84105, Israel

Strategies for controlling the orientation and limiting the defect density in self-assembled structures of copolymers have attracted abiding interest. Using Single-Chain-in-Mean-Field Monte-Carlo simulations and Ginzburg-Landau free-energy computations we study the influence of homogeneous and inhomogeneous electric fields on the self-assembled morphologies of symmetric, lamella-forming copolymer. We present results on the influence of an electric field on the ordering kinetics. We study the interplay between an electric field and a patterned substrate in a thin-film geometry and the relative stability of lamellar phases with different orientations that can form in a cylindric capacitor.

CPP 29.9 Wed 17:45 C 243

microphase behavior and structure of P3HT-b-PPerAcr donor-acceptor block copolymers — Gaurav Gupta[1], Peter Kohn[1], Thomas Thurn Albrecht[1], Michael Sommer[2], Ruth Lohwasser[2], and •Mukundan Thelekkat[2] — [1]Experimental Polymer Phsik, Martin Luther University Halle — [2]Applied Functional Polymers, Macromolecular Chemistry I, University of Bayreuth

Combination of electron and hole conducting organic materials for photovoltaic devices has been an area of extensive research. Short lifetime of the photo generated excitons resulting in diffusion lengths of the order of 10 nm sets a morphological requirement of having nano scale domains. The property of block copolymers to microphase separate into well defined periodic nano structures can be an ideal solution to this morphological requirement as well as for the simultaneous conduction for the dissociated charge carriers. Here we present the structural characterization of a donor *acceptor block copolymer based on side chain poly(perylene-acrylate) as electron conductor and P3HT as hole conductor. Based on scattering measurements we find a molecular weight dependence on the mechanism of microphase separation. While the lower molecular weight polymer showed a transition from a disordered melt at high temperatures to a nanostructured morphology, induced by the crystallization of individual blocks, the higher molecular weight polymer exhibited a microphase separated morphology. The latter remained intact even at low temperatures when crystallization in the individual blocks occurs.

CPP 29.10 Wed 18:00 C 243

Morphological changes during annealing of polyethylene nanocrystals — •Nandita Basu[1], Anna Osichow[2], Stefan Mecking[2], and Günter Reiter[1] — [1]Physikalisches Institut, Albert-Ludwigs Universität Freiburg, Freiburg, Germany — [2]Fachbereich Chemie, Universität Konstanz, Konstanz, Germany

Polymer crystals are metastable and exhibit morphological changes when being annealed. To observe morphological changes on molecular scales we started from small nanometer-sized crystals of highly folded long-chain polymers. Micron-sized stripes consisting of monolayers or stacks of several layers of flat-on oriented polyethylene nanocrystals were generated via evaporative dewetting from an aqueous dispersion. We followed the morphological changes in time and at progressively higher annealing temperatures by determining the topography and viscoelastic properties of such assemblies of nanocrystals using AFM. Due to smallness and high surface-to volume ratio of the nanocrystals, already at 75 °C, i.e. about 60 degrees below the nominal melting point, the lateral size of the crystal coarsened. Intriguingly, this occurred without a noticeable reduction in the number of folds per polymer chain. Starting at around 110 °C, chain folds were progressively removed leading to crystal thickening. At higher temperatures, but still below the melting point, prolonged annealing allowed for surface diffusion of molten polymers on the initially bare substrate which led to the disappearance of crystals. We compared these results to the behavior of the same nanocrystals annealed in an aqueous dispersion and to bulk samples.

CPP 29.11 Wed 18:15 C 243

Two-step nucleation in protein crystallization — •Fajun Zhang[1], Andrea Sauter[1], Marcell Wolf[1], Felix Roosen-Runge[1], Baohu Wu[1], Michael Sztucki[2], Roland Roth[3], Maximilian W.A. Skoda[4], Robert M.J. Jacobs[5], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen — [2]ESRF, France — [3]Universität Erlangen-Nürnberg — [4]ISIS, RAL, UK — [5]CRL, University of Oxford, UK

The attractive forces between proteins in solution are often short-ranged when compared to the size of protein, which can lead to a metastable liquid-liquid phase separation (LLPS) before crystallization. Under these conditions, the order parameters (density and structure) during protein crystal growth can be separately developed leading to a so-called 'two-step' nucleation mechanism. Here we present the results of protein crystallization in solution in the presence of multivalent counterions. It has been shown that negatively charged globular proteins undergo a reentrant condensation phase behavior [1], i.e. a phase-separated regime occurs in between two critical salt concentrations, $c^* < c^{**}$, resulting in a metastable LLPS region. Crystallization near the phase boundaries follows different mechanisms. Close to c*, crystal growth follows the classical nucleation and growth mechanism; close to c**, crystallization follows the two-step mechanism [2]. SAXS measurements demonstrate that protein clusters act as precursors for both the dense liquid phase and nucleation with a reduced energy barrier. [1] F. Zhang, et al., PRL 2008, 101, 148101; Proteins, 2010, 78, 3450. [2] F. Zhang, et al., J. Appl. Cryst. 2011, 44, 755.

CPP 29.12 Wed 18:30 C 243

Kinetics of vesicle formation: A SAXS-stopped-flow study — •Katharina Bressel[1], Michael Muthig[1], Jeremie Gummel[2], Theyencheri Narayanan[2], and Michael Gradzielski[1] — [1]Stranski-Laboratorium, Institut für Chemie, TU Berlin, Germany — [2]European Synchrotron Radiation Facility (ESRF), France

Vesicle formation processes often pass through an intermediate state of disc-like micelles that grow to a maximum size and than close to form vesicles. The driving force for the disc growth is controlled by the line tension of the disc-rim. The balance between the line tension of the discs and the bending elasticity of the vesicle bilayers determines the size and polydispersity of the initially formed vesicles.

In our study we modified the previously studied TDMAO (tetradecyldimethylamine oxide)/LiPFOS (lithium perfluorooctylsulfonate) system by addition of amphiphilic copolymers. The hydrophobic part of these copolymers is incorporated into the surfactant bilayers and is assumed to accumulate in the disc-rim and therefore lower the line tension. That leads to an increase in the maximum size of the disc-like micelles and to a slower vesicle formation. By means of the stopped-flow technique with SAXS detection we studied in situ the kinetics of the vesicle formation process. This rapid-mixing technique allows the observation of kinetic processes in the ms time range and gives excess to detailed structural information about size, shape, and polydispersity of the aggregates. We compared the analysis of these measurements to a coagulation simulation. This simulation is based on a disc growth process that follows a Smoluchowski mechanism.

CPP 30: New Perspectives of Scattering at Soft Matter

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

Invited Talk CPP 30.1 Wed 15:00 C 264

Soft Matter Research at the ESS — •Ken Andersen — European Spallation Source ESS AB, P.O.Box 176, 22100 Lund, Sweden

The European Spallation Source will be a world-leading centre for neutron scattering, based in Lund in Sweden. It will start operation in 2019 and will be fully operational with 22 neutron instruments in 2025. The ESS time structure will be particularly well-suited for cold neutron applications and is expected to outperform existing facilities by at least an order of magnitude. The current status of the project, as well as the plans for instruments and support labs, particularly those relevant for soft matter research, will be presented.

CPP 30.2 Wed 15:30 C 264

Neutron spin echo instrumentation for the European Spallation Source — •Stefano Pasini and Michael Monkenbusch — Forschungszentrum Jülich, 52425 Jülich, Germany

Neutron spin echo (NSE) is the technique with the highest energy resolution for probing the dynamics of materials. At the European Spallation Source (ESS) three different instrument concepts are currently being developed together with Research Center Jülich and the Technical University of Munich. These are a high-resolution spin-echo spectrometer, a wide-angle spin-echo spectrometer and a combined MIEZE and neutron-resonance spin-echo spectrometer. We will present here the progress made in adapting the high-resolution spin-echo spectrometer to the ESS parameters. One part of the work is focused on the specification and conceptual layout of an optimized beam transport including polarization, frame-overlap choppers and avoidance of the direct view. These aspects are quite common between high-resolution and wide angle instrument. Besides the beam transport, the proper spin-echo part consists of magnetic fields for the manipulation of the spin state evolution. Some results on the specification and on the optimization of the magnetic layout of the NSE will be presented.

CPP 30.3 Wed 15:45 C 264

Development of Direct Geometry Chopper spectrometers for the European Spallation Source — •Nicolo' Violini[1], Jorg Voigt[1], Thomas Bruckel[1], Margarita Russina[2], Katharina Rolfs[2], Giovanna Simeoni[3], Wiebke Lohstroh[3], Luca Silvi[3], and Pascale Deen[4] — [1]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Sciences, Leo Brandt Strasse, 52425 Jülich, Germany — [2]-Zentrum Berlin für Materialien, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [3]Technische Universität München, Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II) Lichtenbergstrasse 1, 85747 Garching, Germany — [4]European Spallation Source ESS AB, Box 176, 22100 Lund, Sweden

The long pulse of the ESS will provide a high neutron flux, comparable to the best existing steady state reactors. The main challenge in the instrument design at the future ESS is how to take full advantage of the high neutron peak flux and at the same time to take control over the pulse parameters to best suit the instruments and individual experiments. It has been shown that in particular direct geometry time of flight spectrometers using cold neutrons profit strongly from the long pulse at ESS. In addition the implementation of novel multiplexing techniques, such as RRM and WFM will allow the multispectral instruments to better exploit the source features. Within the German ESS Design Update Phase, we will present the recent progress in the Work Package I1 on chopper spectroscopy. We describe the main aspect of the instruments design, especially focusing on the purpose to achieve a high energy resolution (<0.5%) and its implications.

CPP 30.4 Wed 16:00 C 264

Dynamics in an enzyme containing bicontinuous microemulsion: A quasielastic scattering study — Ralph Neubauer[1], Stefan Wellert[2], Andreas Richardt[3], Marc-Michael Blum[4], and •Thomas Hellweg[1] — [1]Phys. und Biophys. Chemie (PC III), Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany — [2]Stranski Lab. f. Physikalische und Theoretische Chemie, TU Berlin, Straße des 17. Juni 124, 10623 Berlin, Germany — [3]WIS Munster, ABC-Schutz, Humboldtstraße 100, 29633 Munster, Germany — [4]Blum-Scientific Services, Ledererstraße 23, 80331 Munich, Germany

The enzyme diisopropyl fluorophosphatase (DFPase) from the squid *Loligo vulgaris* is of relevance due to its ability to catalyze the hydrolysis of highly toxic organophosphates. In the present work, the enzyme structure in solution (native state) is studied by different scat-

tering methods. The results are compared to hydrodynamic model calculations. Bicontinuous microemulsions (bME) made of sugar surfactants are discussed as reaction media for the DFPase. The bME remains stable in the presence of the enzyme, which is revealed by scattering experiments. It is shown that the DFPase still has a high activity in the bME [1]. The collective and the local motion of the surfactant interface in the bME is studied by means of neutron spin-echo. Moreover, it is tried to study the enzyme motion decoupled from the microemulsion by contrast variation.
[1]S. Wellert, B. Tiersch, J. Koetz, A. Richardt, A. Lapp, J. Gäb, O. Holderer, M.-M. Blum, C. Schulreich, R. Stehle und T. Hellweg; European Biophys. J., 40:761–774, 2011.

CPP 30.5 Wed 16:15 C 264

Chain dynamics of n-alkanes studied by neutron scattering and MD simulations — •Humphrey Morhenn[1], Sebastian Busch[1], and Tobias Unruh[2] — [1]Physik Department E13 and Forschungs-Neutronenquelle Heinz-Maier-Leibnitz (FRM II), Technische Universität München, 85747 Garching, Germany — [2]Lehrstuhl für Kristallographie und Strukturphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

The analysis of local molecular dynamics on time scales shorter than the long-range diffusion relaxation time is challenging. Quasielastic neutron scattering probes the dynamics on a molecular length and a picosecond time scale. Corresponding data was used to validate MD simulations of liquid hexadecane with respect to the short time dynamics. From the analysis of the MD simulations a detailed picture of the local molecular motions in the liquid could be gained. It is e.g. possible to distinguish and specify local torsional dynamics and global rotational diffusion of the molecules. Using this information a physical model describing the short time motion of medium chain molecules is being developed.

CPP 30.6 Wed 16:30 C 264

Influence of the Incident Wavelength on the Apparent Diffusion Coefficient of Au Nano Rods — •Maryam Haghighi[1], Makus Plum[1], Georgios Gantzounis[3], George Fytas[1,2], Hans-Jürgen Butt[1], and Werner Steffen[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Department of Material Science, University of Crete, Heraklion, Greece — [3]University of Athens, Section of Solid State Physics, Athens, Greece

Depolarized dynamic light scattering is a powerful method to measure the diffusion and the rotation of anisotropic particles in solution [1]. Compared to free diffusion in bulk solution, movement close to an interface is influenced by several factors, e.g. hydrodynamic or electrostatic double layer forces. To investigate the dynamics of nanoparticles close to an interface Resonance Enhanced Dynamic Light Scattering (REDLS) is employed [2]. We investigate the diffusion as well as the rotation of Au nano rods in bulk and compared to experiments performed with REDLS close to the solid-liquid interface. Our results show an alteration of the apparent diffusion coefficient of the Au nano rods depending on the incident wavelengths and on the aspect ratio of Au nano rods in bulk solution. We attribute these non-intuitive results to the interplay of surface plasmons generated at certain wavelength in the nano rods themselves and the incident field for the light scattering experiment. [1] Berne, B.J. and Pecora, R., Dynamic light scattering with applications to chemistry Biology and physics (Dover, 2000) [2] Plum M. A., Steffen W., Fytas G., Knoll W. and Menges B., Optics Express 17:10364, 2009

15 min break

Invited Talk CPP 30.7 Wed 17:00 C 264

Scanning small-angle X-ray scattering: Imaging nano-scale properties of extended samples — •Oliver Bunk — Paul Scherrer Institut, Swiss Light Source, 5232 Villigen PSI, Switzerland

Small-Angle X-ray scattering (SAXS) is sensitive to the average nanoscale structure within the illuminated area. With the advent of 3rd generation synchrotron radiation undulator beamlines, X-ray optics of adequate quality and fast, low noise, high dynamic range 2D X-ray detectors scanning SAXS turned from a proof-of-principle to a routinely applied imaging technique, applied in 2D and 3D. It allows imaging nano scale structures over extended, square centimeter sized areas.

After a brief introduction to the technique examples will be shown that include the detection of melt-flow induced alignment in injection moulding of polymers, carbon nanotube reinforced polycarbonate as a two-component system and examples from the biomedical field like bone and brain research that hint at future applications of this technique in the field of soft matter research.

CPP 30.8 Wed 17:30 C 264

Resonant Soft X-Ray Reflectivity - A tool to study the near-surface structure of complex liquids — •Markus Mezger[1], Benjamin Ocko[2], Harald Reichert[3], and Moshe Deutsch[4] — [1]Max-Planck-Institut für Polymerforschung, Mainz — [2]Brookhaven National Laboratory, Upton NY, USA — [3]European Synchrotron Radiation Facility, Grenoble, France — [4]Bar-Ilan University, Ramat-Gan, Israel

X-ray reflectivity (XRR) became one of the leading techniques to study the near-surface structures of liquids. However, standard XRR is not atom-specific and can determine only surface-normal total electron density profiles. In complex liquids, this generally leads to ambiguities in the assignment of molecular moieties to reconstructed interfacial profiles. Resonant x-ray scattering techniques can overcome this limitation by enhancing and modulating the scattering contrast between different molecular moieties.

We present the first fluorine K-edge resonant soft-XRR study of the surface structure of a complex fluid, the ionic liquid $[\mathrm{C_{18}mim}]^+[\mathrm{FAP}]^-$. Analysis of the x-ray absorption spectroscopy and resonant XRR data reveal a depth-decaying near-surface layering. The contributions of specific molecular moieties was unambiguously determined with submolecular resolution. Temperature-dependent XRR, SAXS, and FTIR uncover an intriguing melting mechanism for the layered region, where alkyl chain melting drives a negative thermal expansion of the surface layer spacing that has hitherto never been observed for an isotropic liquid.

CPP 30.9 Wed 17:45 C 264

Observing Molecular Reactions via Simultaneous Ultrafast X-ray Spectroscopies and Scattering — •Wojciech Gawelda, Andreas Galler, Enrique Cuna, and Christian Bressler — European XFEL, Albert-Einstein-Ring 19, 22761 Hamburg

Structural dynamics research on chemical and biological systems seeks to extend the use of optical probes to the atomic-scale sensitive tools with either x-ray absorption spectroscopy (XAS) or x-ray (and electron) scattering (XRS). These tools were developed at synchrotron radiation sources, and thus ultimately limited to 50-100 ps time resolution due to the x-ray pulse widths.

We have recently succeeded to extend the capabilities of such laser-x-ray studies towards MHz pump-probe repetition rates at different synchrotron radiation sources, with quasi-static S/N. We studied different Fe-based spin transition compounds, via XAS, but now also with x-ray emission spectroscopy (XES) and XRS in one single setup. XES is sensitive to the actual spin state of the system, and XRS allows investigating the global structural environment of the thermally equilibrated sample. In addition, the electron transfer between a Ru-donor and a Co-acceptor atom was observed via TR-XES in a bimetallic bpy-based Ru-Co complex.

More intense xray pulses from x-ray free electron lasers (XFELs) are required in order to permit simultaneous femtosecond scattering and spectroscopic studies. This was done for the first time in liquid solutions of Fe-based spin transition compounds at the XPP end station of the LCLS, next to a Ru-Co based compound, and results discussed.

CPP 30.10 Wed 18:00 C 264

X-Ray Nano-Diffraction on Intracellular Keratin Bundles — •Britta Weinhausen[1,2], Jannick Langfahl-Klabes[1,2], Christian Olendrowitz[1], Tim Salditt[1,2], and Sarah Köster[1,2] — [1]Institute for X-Ray Physics, University of Göttingen, Germany — [2]Courant Research Centre Nano-Spectroscopy and X-Ray Imaging, University of Göttingen, Germany

The cytoskeleton of eukaryotic cells is a complex network of filamentous biopolymers, which gives cells their versatile shapes and specific mechanical properties. It mainly consists of three different types of filaments: actin filaments, microtubules and intermediate filaments. Keratin intermediate filaments mainly occur in epithelial cells, where they form about 100 nm thick bundles that are organized in a crosslinked network and provide these cells with a high tensile strength as well as the capability to withstand external stresses.

Our goal is to probe the native structure of keratin bundles in live eukaryotic SK8/K18 cells in a physiological environment. For this purpose we use X-ray diffraction with a nanofocused X-ray source, which enables us to achieve high-resolution structural information in combination with a non-destructive sample preparation. Nevertheless, to simplify the experimental set-up, first synchrotron experiments were performed on fixed and freeze-dried cells. High-resolution dark-field contrast image, where the cellular substructure is visible, were obtained and the analysis of single diffraction patterns obtained on keratin bundles showed oriented scattering corresponding to a high degree of orientation in the sample.

CPP 30.11 Wed 18:15 C 264

Investigation of structural changes of polymer surfaces during friction by GISAXS — •Konrad Schneider[1], David Nitsche[1], and Stephan Roth[2] — [1]Leibniz-Institut für Polymerforschung Dresden, Germany — [2]HASYLAB at DESY Hamburg, Germany

The materials behaviour during friction is not yet well understood. On macro-scale mainly the contact between certain points or asperities happens and wear is observed. Measuring on nano-scale by a SFM mainly topography and local stiffness are mapped. By a new friction device we investigate friction between a well-defined glass sphere and a polymer surface. This surface is created by grafting of polymer layers with thickness of some nm on a wafer. Friction is performed in dependence of normal load. The changes in surface morphology were characterized by GISAXS (grazing incidence small angle X-ray scattering). This enables to monitor flattening and destruction of the polymer layer on the surface as well as the creation of certain ripple structures.

CPP 30.12 Wed 18:30 C 264

Millisecond time resolution GISAXS investigation of metal nanoparticle growth on soft and hard surfaces — Ezzeldin Metwalli[1], Volker Körstgens[1], Adelin Buffet[2], Jan Perlich[2], Stephan V. Roth[2], and •Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany

Metal deposition on solid supports and polymer surfaces is of importance in many areas such as metal electrodes and engineered nanomaterials [1]. Here, gold in its atomic state is deposited on both soft homopolymer films and hard silicon surface by utilizing a DC magnetron sputtering deposition system. With the unprecedented time resolution of ten milliseconds, the nucleation/growth dynamics of gold nanoparticles on both surfaces is monitored using in situ real-time grazing incidence small angle x-ray scattering (GISAXS). An initial rapid change of the particle size and shape is detected and a large particle size distribution becomes narrower with increasing the particle size. At silicon surface, metal deposits exhibit heterogeneous distributions and asymmetric nanoparticle growth compared to those on soft polymer film. At high metal load, a smooth and uniform metal layer on the polymer surface is attributed to an initial high particle mobility and bridging interactions between particles. A transient network between the bridges and strong metal-metal interactions may explain the progressive slow dynamics at concentrated metal particle dispersions. [1] Kaune et al. ACS Appl.Mater.Interfaces 3, 1055 (2011)

CPP 31: Organic semiconductors II

Time: Thursday 9:30–12:45 Location: C 130

Invited Talk CPP 31.1 Thu 9:30 C 130

Large area flexible and stretchable electronics — •Siegfried Bauer — Soft Matter Physics, Johannes Kepler Universiry, Altenbergerstrasse 69, A-4040 Linz, Austria

Today's electronics is stiff, usually made of brittle materials. Tomorrow's electronic may be highly flexible and even mechanically deformable to conform to arbitrary forms. Such electronics must be build on a combination of soft and hard materials. Challenges in this field of research are the largely different mechanical properties of the materials used: entropy elastic elastomers and energy elastic solids. New research directions in mechanics emerge leading to new and unexpected electromechanical instabilities. In the presentation, a tour d'horizon through the mechanics of soft materials under extreme conditions of stretch is given. Examples chosen will be based on recent developments in large area flexible and stretchable electronics, such as ultrathin, ultraflexible and ultracompliant organic solar cells, integrated sensors and active matrix arrays. Work supported by the Austrian Science Funds and by the European Research Council under the advanced grant Soft-Map.

CPP 31.2 Thu 10:00 C 130

Doping as a new approach in promoting charge separation in polymer:fullerene solar cells — •Daniel Riedel[1], Felix Deschler[1], Enrico Da Como[1], Jochen Feldmann[1], Bernhard Ecker[2], and Elizabeth von Hauff[2] — [1]PhOG, Department of Physics, LMU, Munich — [2]Institute of Physics, University of Freiburg

Charge separation at polymer:fullerene interfaces is the primary process for organic bulk-heterojunction solar cells. Following the ultrafast photoinduced charge transfer, electrons and holes are still bound because of Coulomb interactions, resulting in the formation of charge transfer excitons (CTEs). Those are known to play a crucial role in solar cells being responsible for the open circuit voltage and the short circuit current. In this contribution, we propose a novel strategy to overcome some of the recombination channels due to charge transfer excitons. This new approach considers the modification of the electronic properties of the conjugated polymer by doping with F4TCNQ molecules. The free holes induced by F4TCNQ on the low-bandgap polymer PCPDTBT fill the tail of states in the highest occupied molecular orbital (HOMO) and in addition are expected to screen Coulomb interactions of CTEs at the interface between PCPDTBT and the fullerene derivative PCBM. By the unique combination of time resolved photoluminescence and photoinduced absorption spectroscopy, we demonstrate how doping results in a decreased population of CTEs and enhanced formation of free carriers. The spectroscopy experiments are complemented by measurements on solar cells showing an overall increase of more than 30% in the power conversion efficiency.

CPP 31.3 Thu 10:15 C 130

Improved performance of organic photovoltaic cells processed on corrugated substrates structured with laser interference patterning — •Reinhard Scholz[1], Lars Müller-Meskamp[1], Yong Hyun Kim[1], Simone Hofmann[1], Karl Leo[1], Sebastian Eckardt[2], and Andrés Fabián Lasagni[2] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden — [2]Fraunhofer Institut für Werkstoff- und Strahltechnik, Dresden

Due to the short exciton diffusion length in organic semiconductors, bulk heterojunction solar cells consisting of donor-acceptor blends can help to improve the charge separation of the photocarriers. However, in the blends, problems in the formation of continuous percolation pathways towards the electrodes limit the total absorber thickness to rather low values, so that the photovoltaic cells would greatly benefit from an improved light management and an optical concentration in the absorber layer. We successfully use direct laser interference patterning (DLIP) to generate periodic surface structures on different types of substrates. DLIP uses high power laser pulses to ablate the target material directly, without need for classical lithography, resist, and transfer steps, allowing instead scalable structuring at reasonable costs and throughput. Comparing photovoltaic cells grown on corrugated substrates with reference cells grown on a flat surface of the same material, we obtain a relative enhancement of the power conversion efficiency by a factor of 1.21 [1].

[1] L. Müller-Meskamp, Y. H. Kim, T. Roch, S. Hofmann, R. Scholz, S. Eckardt, K. Leo and A. F. Lasagni, Adv. Mater. (2011) *in press.*

CPP 31.4 Thu 10:30 C 130

Blocking layer influence on Diindenoperylene based photovoltaic devices — •Andreas Steindamm[1,2], Michael Brendel[1,2], Katharina Topczak[1], and Jens Pflaum[1,2] — [1]Exp. Phys. VI, Julius-Maximilians-University Würzburg, D-97074 Würzburg — [2]ZAE Bayern e.V., D-97074 Würzburg

Diindenoperylene (DIP) has shown to be a suited donor material in combination with the acceptor C_{60} resulting in bilayer photovoltaic cells with open circuit voltages up to 0.9 V. Together with an exceptionally high fill factor of 74 % this yields an overall cell efficiency of around 4 % [1]. However, a severe drawback is the rather poor light absorption of the crystalline DIP layer due to the unfavorable orientation of transition dipoles along the surface normal, i.e. perpendicular to the electric field vector of the incident light. Therefore, harvesting of all photon-generated excitons is essential in these structures to achieve highest photocurrents possible. As a promising concept the application of exciton blocking layers (EBLs) has been suggested and will be addressed in this contribution by means of an intermediate Batho-Phenanthrolin (BPhen) EBL between the fullerene acceptor and the metallic cathode. As a main result, a doubling of the short circuit current (I_{SC}) could be achieved by implementing the BPhen EBL. To identify the underlying effects, responsible for this enhancement, we employed photoluminescence (PL) quenching measurements which allow for separation of contributions caused by exciton reflection versus those related to metal penetration during depositon.

[1] A. Opitz, et al., IEEE J. Sel. Top. Quant. El. 16 (2010) 1707

CPP 31.5 Thu 10:45 C 130

Evidence for non-isotropic emitter orientation in a red phosphorescent OLED and its implications for determining the emitter's radiative quantum efficiency — •Tobias Daniel Schmidt[1], Michael Flämmich[2], Jörg Frischeisen[1], Dirk Michaelis[2], Norbert Danz[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Fraunhofer Institute for Applied Optics and Precision Engineering, 07745 Jena, Germany

The efficiency of organic light-emitting diodes (OLEDs) is still limited as only a fraction of the consumed electrical power is converted into light and only a small part of this light is finally extracted from the device to air. Especially the radiative quantum efficiency (RQE) of the utilized guest-host system is of interest and should be close to unity in phosphorescent emitter/matrix combinations in order to achieve highly efficient devices. We show that the commonly used red phosphorescent emitter $Ir(MDQ)_2(acac)$ doped in an α-NPB matrix exhibits a profound non-isotropic dipole orientation of the emitter molecules. Ignoring this feature leads to a significant overestimation of the RQE or other factors, which determine the external quantum efficiency of a device. Furthermore, we demonstrate the huge potential for efficiency enhancement of mainly parallel dipole emitter orientation in phosphorescent OLED systems.

CPP 31.6 Thu 11:00 C 130

Tailoring the electronic properties of polypyrrole thin films for acid detection — •Céline Vervacke[1], Carlos César Bof Bufon[1], Pablo Roberto Fernández Siles[1,2], and Oliver G. Schmidt[1,2] — [1]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Material Systems for Nanoelectronics, TU Chemnitz, Reichenhainerstrasse 70, 09107 Chemnitz, Germany

Water acidification is one of the most important environmental issues affecting all ecosystems [1]. In this work we demonstrate the fabrication and characterisation of HCl, H2SO4 and H3PO4 detectors based on chemically grown polypyrrole (PPy) thin films with thickness below 100 nm [2, 3]. In addition, the organic layers are incorporated into self-wounded microtubes with diameter of about 15-20 μm for lab-on-a-chip integration. In order to allow the acid detection, PPy was successfully discharged in water, minimizing in this way the polymer degradation which is often observed when performed by other means (e.g. chemical and electrochemical reduction) [4]. The investigation of the structural modifications and the electrical properties were conducted by means of transport measurements, infrared spectroscopy, cyclic voltammetry and current sensing AFM methods.

1. C.D. Evans et al., Environ. Sci. Technol. 45, 1887 (2011)
2. C.C. Bof Bufon and T. Heinzel, Appl. Phys. Lett. 89, 012104 (2006)
3. C.C. Bof Bufon and T. Heinzel, Phys. Rev. B 76, 245206 (2007)
4. C.C. Bof Bufon et al., J. Phys. Chem. B 114, 714 (2010)

15 min break

CPP 31.7 Thu 11:30 C 130

Magnetoresistive organic field-effect transistors based on donor/acceptor blends — •Thomas Reichert, Tobat P. I. Saragi, and Josef Salbeck — Macromolecular Chemistry and Molecular Materials, Department of Mathematics and Science and Center for Interdisciplinary Nanostructure Science and Technology, University of Kassel, Heinrich Plett Strasse 40, D 34132 Kassel, Germany

Room temperature magnetoresistive organic field-effect devices operated at low magnetic fields (<100 mT) are presented. They consist of different coevaporated donor/acceptor blends, with a high probability for intermolecular charge-transfer states. No magnetic field-effect is observed in the devices of pristine compounds. In contrast, a significant magnetoresistance effect is obtained in the mixed systems. The sign of magnetoresistance can be tuned by varying the applied drain and gate voltages. The magnetoresistance values also depend on the composition of the donor- and acceptor-molecules. Our results contribute to the elucidation of the origin of magnetoresistance in organic field-effect transitors and open a way to magnetosensitive organic devices without ferromagnetic materials.

CPP 31.8 Thu 11:45 C 130

Crystal Growth of Organic Compound From The Melt — •Huamin Irvine Hong and Christian Kloc — School of Materials Science and Engineering Nanyang Technological University Block N4.1 Nanyang Avenue Singapore 639798

In this study, single crystals of anthracene up to few centimeters were developed from the melt based on a self designed, inexpensive and versatile zone refining apparatus. Platelets cut from these crystals by applying thread saw were tested for purity and perfection by Powder X-ray Diffraction (XRD), Laser Desorption Ionization-Time of Flight Mass Spectrometry (LDI-ToF MS), Fourier-Transform Infrared Spectroscopy (FT-IR), Atomic Force Microscopy (AFM) & fluorescence measurement. Based on the purity analysis, impurities within commercial anthracene powder such as Carbazole and 9, 9*Bianthryl (dimers) have been reduced significantly as indicated by LDI-ToF MS analysis.

In addition, single crystals of Stilbene up to few centimeters (ideal scintillation properties) has been developed applying the same technique. The Stilbene crystal does not show any formation of intrinsic impurities such as dimers as compared to those of anthracene crystal upon zone refinement. Hence, the results indicate that zone refinement can produce high quality organic crystals with desired properties provided that intrinsic impurities (dimers etc) do not form upon the thermal fusion.

CPP 31.9 Thu 12:00 C 130

Non-empirical Determination of the Fraction of Exact Exchange in Density-functional Theory — •Viktor Atalla[1], Mina Yoon[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Oak Ridge National Laboratory, USA

Calculating the electronic structure of small molecules with density-functinoal theory (DFT) is challenging because conventional exchange-correlation (XC) functionals typically severely underestimates HOMO-LUMO gaps, which may result in a wrong description for charge transfer between weakly interacting molecules.

Here we consider the PBE0 [1] types of XC functionals using the fraction of exact exchange (α) as an adjustable parameter. Employing the G^0W^0 approach we identify the optimum α (α_0) for which the quasi particle correction to the Kohn-Sham HOMO vanishes. We tested this scheme for the G2 datasets of small molecules and find α_0 values in the range of $0.7 - 0.9$. The generalized Kohn-Sham HOMO levels at the α_0 have a mean error of ~ 0.3 eV with respect to the experimental vertical ionization potentials.

We apply the scheme for the prototypical donor-acceptor complex TTF/TCNQ and obtain $\alpha_0 \sim 0.8$, which gives an electronic level alignment consistent with the experimental value. It follows that this system rather exhibits intra-molecular electron-density rearrangement then charge transfer.

[1] C. Adamo, V. Barone, J. Chem. Phys. **110**, 6158 (1999)

CPP 31.10 Thu 12:15 C 130

Ab initio simulations in aza-bodipy derivatives: How energetic disorder affects the charge carrier mobility in 3D systems — •Sebastian Radke, Rafael Gutierrez, Caroline Gollub, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany

Potential candidates for low cost large area photovoltaic applications are organic solar cells based on small molecules because they can be produced on flexible substrates at low temperatures. To enlarge their efficiency, organic absorber materials covering the whole sun light spectrum are required. Nevertheless, efficient infrared absorbers for application in organic solar cells are still rare.

Based on first principle methods, we investigate theoretically the electronic structure and the charge transport of a promising near-infrared absorber material, bis-(phenyl)-borondifluoride-azadiisoindomethene. We simulate the charge carrier mobility in terms of disorder kinetic Monte Carlo simulations by means of semi-classical Marcus theory. By using this approach, we are able to analyze the effects of the dynamics of the electronic system parameters, which are sensitively related to the molecular structure as well as to the system morphology, on the anisotropic charge transport in the different materials. Our theoretical investigations enable us to predict and to understand experimental findings on this material and help to develop a materials design not only for the class of aza-bodipy derivatives but also for arbitrary highly ordered molecular systems.

CPP 31.11 Thu 12:30 C 130

Continuum Solvent Model for extended periodic Systems — •Matthias Witte, Uwe Gerstmann, Eva Rauls, and Wolf Gero Schmidt — Universität Paderborn, Germany

Solvent influences play an important role in physical chemistry and are becoming recently a matter of interest for density functional theory (DFT) [1]. In order to increase the applicability to more realistic systems one needs to combine periodic systems and a solvent model. Periodic boundary conditions are still important for condensed matter systems and surfaces. We implemented the continuum solvent model proposed by Fattebert et al. [2] in the plane wave DFT code PWscf [3]. The modified Poisson equation is solved with the Parallel algebraic MultiGrid (PMG) solver [4]. Instead of the suggested zero-Dirichlet boundary conditions we use a different approximation using the screened Hartree potential. With this approach we studied various physical properties, like e.g. the optical absorption of small model systems in solution and their dependence of the surrounding medium. First test calculations show good agreement with theoretical data.

[1] J. Tomasi et al., Chem. Rev. 105 (2005) 2999
[2] J.L. Fattebert et al., Int. J. Quantum Chem., 23 (2002) 662
[3] P. Giannozzi et al., J. Phys.: Condens. Matter 21 (2009) 395502
[4] M.J. Holst et al., J. Comput. Chem. 14 (1993) 105

CPP 32: Focus: Stress Relaxation in Polymers - From single molecules to biological cells (joint focus with BP)

The session provides a synopsis of stress relaxation in polymeric materials, ranging from synthetic to biological polymers and from single molecule studies to network properties and their relevance for live cells and tissues. (Organizers: R. Magerle, K. Kroy)

Time: Thursday 9:30–12:30 Location: C 243

Invited Talk CPP 32.1 Thu 9:30 C 243

Stress relaxation and chain dynanics in entangled polymer melts — •Ralf Everaers — Laboratoire de Physique, ENS Lyon, 46 allee d'Italie, F-69364 Lyon, France

High molecular weight polymeric liquids display remarkable viscoelastic properties. Contrary to glassy systems, their macroscopic relaxation times are not due to slow dynamics on the monomer scale, but arise from the chain connectivity and the restriction that the chain backbones cannot cross. We use a combination of analytical theory and computer simulations to arrive at a quantitative description of the complex relaxation scenario expected from current versions of the tube model. Our data for the stress relaxation in equilibrium and step-strained bead-spring polymer melts allow us to explore the chain dynamics and the shear relaxation modulus, $G(t)$, into the plateau regime for chains with $Z = 40$ entanglements and into the terminal relaxation regime for $Z = 10$. We have performed parameter-free tests of several different tube models using the known (Rouse) mobility of unentangled chains and the melt entanglement length determined via the primitive path analysis of the microscopic topological state of our systems. We find excellent agreement for the Likhtman-McLeish theory using the double reptation approximation for constraint release, if we remove the contribution of high-frequency modes to contour length fluctuations of the primitive chain. In particular, we rationalize the onset of entanglement constraints in polymeric liquids via an analysis of the short-time dynamics of (primitive) chains.

CPP 32.2 Thu 10:00 C 243

Direct stress measurements in nonequilibrium thin polymer films. — •Katherine Thomas[1] and Ullrich Steiner[2] — [1]Max Planck Insitute for Dynamics and Self-Organisation, Goettingen, Germany — [2]Department of Physics, University of Cambridge, UK

Residual stresses in polymer films often arise from the solution deposition protocol. The origin of stresses in polymer films is easily justified: film formation by solvent evaporation steadily increases the polymer concentration, raising the glass transition temperature of the solution. When Tg reaches the ambient temperature the polymer vitrifies, suppressing further equilibration of the chains. Due to the entangled nature of the polymer network, evaporation of the remaining solvent induces substantial biaxial tensile stresses. Stresses in thin films are not, however, easy to measure and can often only be deduced indirectly.

Here stresses were quantitatively determined by measuring the deflection of cantilevers cut from film-covered SiN membranes using a focused ion beam. Spin-cast films showed notably high residual stresses, far greater than the bulk polymer tensile strength. Stress relaxation via thermal annealing suggests two relaxation mechanisms, both much faster than the reptation time. The fast relaxation indicates that the stress arises from segmental deformations of the chains, rather than entropic effects. Comparison of these data with EHD film stability experiments, suggests the same relaxation mechanisms, providing further evidence for the existence of a thin, highly stressed layer at the surface of the film. These experiments show the utility of our method for the systematic examination of non-equilibrium thin film properties.

CPP 32.3 Thu 10:15 C 243

Mechanical stress relaxation in polymers followed by low-field NMR — Ute Böhme and •Ulrich Scheler — Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany

Low-field NMR provides information on molecular mobility over a wide range of rates of motion. In-situ low-field NMR has been applied on polymers under uniaxial stress [1]. Strongest stress-induced effects have been observed in T2 (indicative for slow motion) and T1rho (indicative for mtion of rates of kilohertz) both indicating restictions in the motion of polymer segments. In elastomers the changes a reversible after release of the external stress. Time-dependent experiments at constant extension on semicrystalline polymers show a return of both relaxation times to the values of the non-stressed sample. However, the time constant of that return is significantly longer than that observed in mechanical stress-relaxation experiments.

[1]Böhme, U.; Gelfert, K.; Scheler, U. Solid-state NMR of polymers under mechanical stress AIP conference proceedings 1330 (2011) 109

CPP 32.4 Thu 10:30 C 243

Stress Induced Single Molecule Reorientation Motion in Elastomeric Polypropylene — •Stefan Krause, Martin Neumann, Melanie Bibrach, Robert Magerle und Christian von Borczyskowski — Fakultät für Naturwissenschaften, TU Chemnitz, D-09107 Chemnitz

The fluorescence of a single molecule (SM) is a very sensitive probe for its environment and changes of the fluorescence lifetime, emission wavelength, and polarization can report spatial and temporal variations in the surrounding structure of the fluorescent dye. Here we report on SM microscopy and spectroscopy studies of stress relaxation in thin films of elastomeric polypropylene (ePP), a semicrystalline polymer with a complex microstructure of crystalline and amorphous regions on the nanometer scale. The films are stretched using a micro tensile testing setup. Simultaneously, perylenediimide dyes functionalized with hexadecane were embedded in the ePP film and report via their molecular dynamics changes within their local environment. Orientation fluctuations were investigated via SM polarization dependent microscopy. This experiment allows for insights into dynamical processes within the amorphous regions of ePP which are not accessible using other microscopy techniques.

Invited Talk CPP 32.5 Thu 10:45 C 243

Slow stress relaxation in recoiling polymers — •Ulrich F. Keyser — Cavendish Lab, University of Cambridge, JJ Thomson Ave, Cambridge, CB3 0HE, UK

The internal dynamics of semi-flexible chains in response to external forces is an important problem in soft matter, polymer and biological physics. Here, we describe a novel method to experimentally determine the relaxation of a single DNA molecule with one free end. The electric field in a nanopore[1] or nanocapillary[2] is used to apply a controlled force to one end of a DNA molecule while the other end is held in an optical trap[3,4]. High-speed video tracking of the colloidal particle[5] allows for a direct measurement of the relaxation in the recoiling DNA upon release from the nanopore. We show and discuss our single-molecule experiments for a range of forces and find that stress relaxation and recoiling is much slower than expected from the simple worm-like chain model. Our results pave the way towards investigating the nonlinear dynamics of semiflexible polymer relaxation and test recent theories[6] on propagation and relaxation of backbone tension in DNA.

[1] Keyser et al., Nature Physics 2, 473 (2006) [2] Steinbock et al., Nano Letters 10, 2493 (2010) [3] Steinbock et al., J. Phys. Cond. Mat. 23, 184114 (2010) [4] Otto et al., Rev. Sci. Instr. 82, 086102 (2011) [5] Otto et al., Optics Express 18, 22722 (2010) [6] Hallatschek et al., Phys. Rev. E 75, 031906 (2007)

CPP 32.6 Thu 11:15 C 243

Non-Equilibrium Relaxation in Polymer Solutions — •Chien-Cheng Huang, Gerhard Gompper, and Roland G. Winkler — Theoretical Soft Matter and Biophysics, Institute of Complex Systems and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich

Individual DNA molecules in shear flow exhibit large conformational changes due to tumbling motion. A polymer continuously undergoes stretching and compression cycles with a characteristic frequency, which depends on the shear rate. To characterize the tumbling behavior, we perform large-scale non-equilibrium mesoscale hydrodynamic simulations of semidilute polymer solutions, which combine molecular dynamics simulations and the multiparticle collision dynamics approach. The non-equilibrium polymer end-to-end vector relaxation times in the stationary state exhibit the shear rate dependence $\dot{\gamma}^{-2/3}$. In the dilute limit, the relaxation times for the various spatial directions are identical. For semidilute solutions, screening of hydrodynamic interactions leads to a slower and faster relaxation in the vorticity and gradient directions, respectively. The relaxation times are equal to the tumbling times extracted from cross-correlation functions of fluctuations of radius-of-gyration components. Furthermore, we find a memory effect in the tumbling dynamics, which causes an oscillatory relaxation along the flow and gradient directions. This memory effect decreases with increasing polymer length and is believed to be less pronounced or even absent for long polymers.

CPP 32.7 Thu 11:30 C 243

Stress relaxation through crosslink unbinding in biopolymer assemblies — •Claus Heussinger — Institute for theoretical physics, University Göttingen

The cytoskeleton is a complex meshwork of long elastic filaments coupled together with the help of numerous, rather compact crosslinking proteins. An important aspect of a cytoskeletal polymer network is its dynamic nature, which allows it to react to external stimuli and adapt its internal structure and mechanical properties according to the needs of the cell. The reversible nature of crosslink binding is an important mechanism that underlies these dynamical processes.

In this contribution we devise a simple model polymer network to study the effect of network deformation on the crosslink binding processes. We evidence a discontinuous and sudden rupture transition after which the network is no longer able to resist the external load. By combining MC simulation with a necklace-type model (M. Fisher, J. Stat. Phys. (1984)) we discuss the role of the mechanical stiffness of the crosslinks and the fluctuation properties of the filaments. This allows to address the interplay of strain stiffening inherent in the entropic response of individual polymers, and strain softening due to crosslink unbinding.

CPP 32.8 Thu 11:45 C 243

Thermorheology of single living cells — •Tobias R. Kiessling, Anatol W. Fritsch, Roland Stange und Josef Käs — Universität Leipzig, Institut für Experimentelle Physik I, Physik der weichen Materie, Linnéstr. 5, 04103 Leipzig

Within reasonable temperature ranges, many biological functions are known to undergo modulations, like myosin motor activity, CO2 uptake of cultured cells or sex determination of several species. As mechanical properties of living cells are considered to play a key role for plenty of cell functions ranging from stem cell differentiation to cancer progression, it is surprising that only little is known on how their rheology is affected by temperature. Using an Optical Stretcher, thousands of single cell experiments were performed to systematically assess the effect of temperature on cell deformability. The impact of slow temperature changes occurring on a scale of about 30 minutes is compared to the influence of defined heat shocks in a range of milliseconds. Differences of thereby revealed temperature dependencies are discussed and compared to findings from in vitro rheological studies on polymer solutions.

Invited Talk CPP 32.9 Thu 12:00 C 243

Cytoskeletal stress in collective cell migration — •Xavier Trepat — Institute for Bioengineering of Catalonia, Barcelona, Spain

For a group a living cells to migrate cohesively, it has long been suspected that each constituent cell must exert physical forces not only upon its extracellular matrix but also upon neighboring cells. I will present the first comprehensive maps of these distinct force components. These maps reveal an unexpectedly rich physical picture in which the distribution of physical forces is dominated by heterogeneity, both in space and in time, which emerges spontaneously propagates over great distances, and cooperates over the span of many cell bodies. Both in epithelial and endothelial cell sheets, these heterogeneous forces are mechanically linked to cell velocities through a newly discovered emergent mechanism of innately collective cell guidance: plithotaxis.

CPP 33: Polymer Dynamics

Time: Thursday 9:30–12:30 Location: C 264

Topical Talk CPP 33.1 Thu 9:30 C 264

Neutron Scattering Studies on Self-Healing Model Polymers — •Ana Rita Brás[1], Jessalyn Cortese[2], Corinne Soulié-Ziakovic[2], François Tournilhac[2], Jürgen Allgaier[1], Wim Pyckhout-Hintzen[1], Andreas Wischnewski[1], Ludwik Leibler[2], and Dieter Richter[1] — [1]Forschungszentrum Jülich, JCNS-1/ICS-1, D52425 Jülich, Germany — [2]Matière Molle et Chimie, ESPCI-CNRS (UMR7167), France

Supramolecular polymers are an increasingly important class of polymers, where designed intermolecular interactions allow a specific tailoring of polymer properties. One of the most recent additions to this field are self-healing polymers, which base on the hydrogen-bonding interaction of groups on parts of the molecules. Neutron scattering measurements were performed on recently synthesized model systems, using DNA-inspired end-groups like Thymine-1-acetic acid, Diaminotriazine and 2-aminoethyl-imidazolidone with properties closer to natural materials. The backbone was polypropylene(glycol) and polyethylene(glycol) based polymer, respectively. The end-functionalization allowed going from one to three reactive sites, shifting the association equilibrium to bonding. Both Small Angle Neutron Scattering and Neutron Spin-Echo allowed to quantitatively access the assembly process thus probing the hydrogen-bonding association mechanism. Results of these measurements will be presented. For the first time such an association process was observed on quasielastic neutron scattering time scale.

CPP 33.2 Thu 10:00 C 264

Orientation autocorrelation function of the 2nd Legendre polynomial for Rouse chains with fixed ends — •Semjon Stepanow and Kay Saalwächter — Martin-Luther-Universität

Halle-Wittenberg, Institut für Physik, D-06099 Halle, Germany

We have calculated the autocorrelation function of the 2nd Legendre polynomial of the segmental orientation for a Rouse chain with fixed ends. This function is relevent for nuclear magnetic resonance (NMR) measures of chain dynamics in polymer networks [1] and entangled melts [2], for which a chain with fixed ends represents the simplest model for the time range from the segmental relaxation time up to the onset of cross-link or tube constraints. The time-dependent part of the ACF is given by $c_1 t^{-1/2} + c_2 t^{-1}$. It thus deviates from free-Rouse result $\sim t^{-1}$, and compares favorably with experimental data [1,2].

[1] K. Saalwächter, A. Heuer, Macromolecules 39 (2006) 3291

[2] A. Herrmann, V. N. Novikov, and E. A. Rössler, Macromolecules 42 (2009) 2063; F. Vaca Chavez, K. Saalwächter, Phys. Rev. Lett. 104 (2010) 198305

CPP 33.3 Thu 10:15 C 264

Viscoelastic hydrodynamic interactions explain anomalous CM diffusion in polymer melts — •Hendrik Meyer, Jean Farago, and A.N. Semenov — Institut Charles Sadron, CNRS, 67034 Strasbourg, France

Contrary to common belief, hydrodynamic interactions in polymer melts are *not screened* beyond the monomer length and are important in transient regimes. We show that viscoelastic hydrodynamic interactions (VHI) lead to anomalous dynamics of a tagged chain in an unentangled melt at $t < t_N$, the Rouse time. The center-of-mass (CM) mean-square displacement is enhanced by a large factor increasing with chain length. We develop a theory of VHI-controlled chain dynamics yielding a negative CM velocity autocorrelation function which agrees with our molecular dynamics simulations without any fitting parameter. It is shown that Langevin friction strongly affects the short-t CM dynamics, also captured by our theory. All results apply also to entangled melts for times shorter than the entanglement time. Transient VHI effects thus provide the dominant contribution to the subdiffusive CM motion universally observed in simulations and experiments. [Phys. Rev. Lett. 107, 178301 (2011)]

CPP 33.4 Thu 10:30 C 264

Origin of the β-relaxation in Poly(ϵ-caprolactone) — •Björn Kuttich, Christina Lederle, and Bernd Stühn — TU Darmstadt, Experimentelle Physik kondensierter Materie

Broadband Dielectric Spectroscopy is a simple but highly informative measuring method to study polymer dynamics in the bulk as well as under confinement on a large timescale. By analysing the observable dielectric relaxations it is possible to investigate cooperative phenomena like the α-process and also much faster local chain dynamics.

Poly(ϵ-caprolactone) (PCL) is a polymer widely used in engineering and medical engineering. The latter especially because of its biodegradability. Despite of its wide application area, the basic principles of the polymer's dynamics are not yet fully understood. There are only few publications existent in which the mechanic and dielectric relaxations of PCL were investigated. Notably the reasons for the observed dielectric β-relaxation are discussed controversially.

Our experiments are now suited to clarify the reasons for the reported dielectric β-relaxation in bulk PCL. The experiments show a linear dependency of the relaxation strength of the β-relaxation from the amount of water inside the polymer. Furthermore they suggest that this relaxation is completely due to the dynamics of water molecules strongly bound to the PCL by hydrogen bonds which act as small side chains. The comparison to the dynamics of polyamides is in our view ineligible, because PCL lacks the possibility to build intra- or interchain hydrogen bonds in the absence of water molecules.

CPP 33.5 Thu 10:45 C 264

Excitation Dynamics in Donor-Acceptor Copolymers — •B. Gieseking[1], B. Jäck[1], E. Preis[2], S. Jung[2], M. Forster[2], U. Scherf[2], C. Deibel[1], and V. Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — [2]Macromolecular Chemistry and Institute for Polymer Technology, Bergische University of Wuppertal, D-42097 Wuppertal — [3]Bavarian Centre for Applied Energy Research (ZAE Bayern), D-97074 Würzburg

Recently the efficiency of organic bulk heterojunction solar cells could be significantly increased by using donor–acceptor type copolymers in the active device layer. Nevertheless only little is known about the elementary processes following photoexcitation of these materials.

Here we present an in-depth study of the excitation dynamics in the copolymer PCDTBT. By carrying out comparative steady state absorption and photoluminescence (PL) measurements on PCDTBT and its building blocks we assign the two prominent absorption bands to two spatially separated co-monomer units on the polymer chain coupled by an efficient energy transfer process. The relaxation dynamics investigated by time-resolved PL spectroscopy are dominated by a redshift of the spectrum while adding PC$_{70}$BM results in an efficient PL quenching. We find no evidence for a direct decay pathway from the higher energy band of the donor towards the acceptor. Our findings indicate that effective coupling between copolymer building blocks leading to the energy transfer between comonomer units governs the photovoltaic performance of the blends.

15 min break

Topical Talk CPP 33.6 Thu 11:15 C 264

Shear inversion of polymer-brush bilayers with embedded colloids — •Torsten Kreer[1] and Andre Galuschko[2] — [1]Leibniz-Institut fuer Polymerforschung Dresden e.V., Hohe Strasse 6, 01069 Dresden — [2]Institut fuer Theoretische Physik, Georg-August Universitaet, 37077 Goettingen

Based on a recent scaling approach to describe the shear motion of polymer-brush bilayers at constant velocity, the response of bilayers with colloidal inclusions to highly non-stationary inversion processes is discussed by means of molecular dynamics simulations and scaling theory. Bilayers with a simple (dimeric) solvent reveal an overshoot for the shear stress, while simulations of dry brushes without explicit solvent molecules fail to display this effect. For the first time, it is demonstrated that mechanical instabilities can be controlled by the inclusion of macromolecular structures, such as colloids of varying softness. A characteristic time for conformational and collective responses under highly non-stationary shear is introduced. It can be expressed in terms of the equilibrium properties of the bilayer.

CPP 33.7 Thu 11:45 C 264

Rigid vs flexible polyelectrolytes: Structural forces and rheology in nm scale volume — •Cagri Üzüm and Regine v. Klitzing — Stranski-Laboratorium, Institut für Chemie, TU Berlin, Strasse des 17.Juni 124, 10623 Berlin, Germany

In this contribution, flexible and rigid polyelectrolytes (i.e. NaPSS and DNA) in aqueous medium are compared with respect to two small scale dynamic parameters. First, the existence and dynamics of oscillatory structural forces in confinement were studied by colloidal probe AFM. In accord with theoretical calculations, structural forces are suppressed with increasing chain rigidity, presumably due to a longer chain reorientation time in the confinement [1].

Second parameter is the newly introduced micro-viscosity, which corresponds to the viscosity in nm scale volumes. It was measured by an AFM microcantilever [2]. While the solutions of flexible chains have nearly the same micro-viscosity as the bulk, rigid chains have significantly lower ones as compared to the bulk viscosity. Possible reasons for this significant difference are addressed.

[1] Kleinschmidt, F.; Stubenrauch, C.; Delacotte, J.; von Klitzing, R. and Langevin, D. J. Phys. Chem. B, (2009), 113, 3972-3980

[2] Boskovic, S.; Chon, J.; Mulvaney, P. and Sader, J. J. Rheol., (2002), 46, 891-899

CPP 33.8 Thu 12:00 C 264

Time-Humidity-Superposition Principle in Conductivity Spectra of Ion-Conducting Polymers — Cornelia Cramer[1], Souvik De[1,2], and •Monika Schönhoff[1] — [1]Institute of Physical Chemistry, University of Muenster, Corrensstraße 28/30, 48149 Münster, Germany — [2]Graduate School of Chemistry, University of Muenster, Corrensstraße 28/30, 48149 Münster, Germany

We analyze the scaling properties of the ac conductivity spectra of ion-conducting polyelectrolyte complexes (PEC) of different compositions. PEC are composed of cationic poly(diallyldimethyl ammonium chloride)(PDADMAC) and anionic poly(sodium 4-styrene sulfonate) (NaPSS) and pressed into dry, solid pellets. Frequency-dependent spectra were taken at ambient temperature but at different relative humidities.

Enhanced humidity increases the long range transport (dc conductivity) as well as the local motions, characterised by the onset of conductivity dispersion. Even more, the complete spectral shape of spectra taken at different humidity can be superimposed to a mastercurve. Thus, for the first time, we report on a scaling principle for conductivity spectra termed 'time-humidity-superposition principle' in analogy with the well-known time-temperature-superposition principle. This model-free scaling holds for different materials over several decades in frequency. It implies that the hydration is activating ion motion over short and long distances in a similar, general way, a concept so far only established for thermal energy.

(1) Cramer, De, Schönhoff Phys. Rev. Lett. 107, 028301 (2011)

CPP 33.9 Thu 12:15 C 264

Lithium transport mechanism in ternary mixtures of polymer electrolytes and ionic liquids - a molecular dynamics simulation study — •Diddo Diddens[1,2] and Andreas Heuer[1,2] — [1]Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster, Germany — [2]Graduate School of Chemistry, Münster, Germany

Electrolytes based on mixtures of lithium salts and poly(ethylene oxide) (PEO) are important candidates for modern lithium ion batteries. Unfortunately, in case of the common binary electrolytes like PEO/lithium-bis(trifluoromethane sulfonimide) (LiTFSI), the ionic conductivity is still too low for an efficient technological use. Here, the incorporation of room temperature ionic liquids (RTILs) into these materials promises a significant improvement, as the ionic conductivity is increased about an order of magnitude at room temperature, thus making them an ideal compromise between solid and liquid electrolytes.

Motivated by these experimental findings, we study the underlying microscopic transport mechanisms of the lithium ions by means of MD simulations. We find that these mechanisms are qualitatively the same as already observed in a previous study for PEO/LiTFSI. When adding ionic liquid into the electrolyte, the characteristic time scale of one of the mechanisms, namely the cooperative motion with the PEO segments, is reduced significantly. Therefore, it is possible to describe the lithium dynamics by a Rouse-based analytical transport model that has been developed for binary polymer electrolytes.

CPP 34: Colloids and Complex Liquids II

Time: Thursday 15:00–18:45 Location: C 130

Invited Talk CPP 34.1 Thu 15:00 C 130

Colloidal quasicrystals: from their discovery to photonic applications — •Stephan Förster[1], Alexander Exner[1], Sabine Rosenfeldt[1], Jan Perlich[2], and Peter Lindner[3] — [1]Physikalische Chemie I, Universität Bayreuth, 95440 Bayreuth, Germany — [2]HASYLAB/DESY, 22607 Hamburg, Germany — [3]Institut Laue Langevin, 38042 Grenoble, France

Micelles are the simplest example of self-assembly found in nature. As many other colloids, they can self-assemble in aqueous solution to form ordered periodic structures. These structures so far all exhibited classical crystallographic symmetries. Using small-angle neutron and x-ray diffraction, for the first time quasi-crystalline micellar phases were observed exhibiting 12-fold and 18-fold diffraction symmetry. Colloidal water-based quasicrystals are physically and chemically very simple systems. This discovery is of particular importance, as it opens a new versatile route to quasicrystalline photonic band gap materials via water-based colloidal self-assembly techniques.

CPP 34.2 Thu 15:30 C 130

Regular packings on periodic lattices — •Tadeus Ras[1,3], Rolf Schilling[1], and Martin Weigel[1,2] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany — [2]Applied Mathematics Research Centre, Coventry University, England — [3]Present address: Fachbereich Physik, Universität Konstanz, Germany

We investigate the problem of packing identical hard objects on regular lattices in d dimensions. Restricting configuration space to parallel alignment of the objects, we study the densest packing at a given aspect ratio X. For rectangles and ellipses on the square lattice as well as for biaxial ellipsoids on a simple cubic lattice, we calculate the maximum packing fraction $\varphi_d(X)$. It could be proved to be continuous with an infinite number of singular points $X_\nu^{\min}$, $X_\nu^{\max}$ $\nu = 0, \pm1, \pm2, \ldots$. In two dimensions, all maxima have the same height, whereas there is a unique global maximum for the case of ellipsoids. The form of $\varphi_d(X)$ is discussed in the context of geometrical frustration effects, transitions in the contact numbers and number theoretical properties. Implications and generalizations for more general packing problems are outlined [1].

[1] T. Ras, R. Schilling and M. Weigel, Phys. Rev. Lett. **107**, 215503 (2011)

CPP 34.3 Thu 15:45 C 130

Fluid-mediated gelation of hard spheres — •Andrea Fortini — Theoretische Physik II, Physikalisches Institut, Universität Bayreuth, Universitätsstraße 30, D-95440 Bayreuth, Germany

We propose a minimal model for the description of the fluid-mediated gelation of purely repulsive colloidal particles described in recent experimental work [Koos, E. and Willenbacher, N. (2011). Science, 331, p.897]. We find that the addition of non-wetting fluid droplets to a suspension of pure hard spheres can lead to the formation of clusters that can eventually percolate and form a gel. We show with Brownian dynamics computer simulations of a binary mixture of colloids and droplets that gelation is due to a percolation transition compatible with diffusion limited cluster aggregation and that the dynamical and mechanical properties are those of a gel of colloidal particles.

CPP 34.4 Thu 16:00 C 130

Hard sphere crystals and crystal-liquid interfaces — •Martin Oettel — Mainz University, Institute of Physics

Density functional theory in the form of Fundamental Measure Theory (FMT) is capable of describing hard sphere crystals and interfaces very accurately. With FMT as a benchmark, we discuss the merits and shortcomings of simpler and more popular models (Ramakrishnan-Youssouff and Phase Field Crystal model). Furthermore we address the concept of crystallinity modes and the associated order parameter profiles at crystal-liquid interfaces as these are central ingredients for coarse-grained phase-field modelling employed in materials science.

CPP 34.5 Thu 16:15 C 130

Fixing contact angles in model colloid-polymer mixtures — •Antonia Statt, Alexander Winkler, Peter Virnau, and Kurt Binder — Institute of Physics, JGU Mainz , 55128 Mainz

We study a continuous version of the Asakura-Oosawa model with grandcanonical simulations as a model system for colloid-polymer mixtures. By applying a novel computational scheme with a "mixed Hamiltonian" the system is slowly driven from bulk to planar confinement and vice versa, and we are able to determine interfacial free energies with respect to walls and contact angles. By varying the colloid-wall interaction range while leaving the polymer-wall interaction constant, we are able to fix arbitrary contact angles ranging from complete wetting of colloids to complete wetting of polymers at the wall. These investigations may not only guide future experiments but also form the basis for the study of heterogeneous nucleation in complex geometries such as cylindrical and spherical confinement.

CPP 34.6 Thu 16:30 C 130

Two-dimensional percolated networks induced by an uniform external field. — •Heiko Schmidle[1], Carol K. Hall[2], Orlin D. Velev[2], and Sabine H. L. Klapp[1] — [1]Technische Universität Berlin — [2]North Carolina State University

In this work we present results of a theoretical investigation of induced dipoles mixed with particles that contain two induced dipoles, one pointing into the field and the other one opposite to it. Our model is based on current experimental works where such particles are synthesized and interesting self-assembly is observed [1]. Induced dipoles tend to form chains into the external field direction [2]. Particles that contain two dipole moments are similar to quadrupolar particles and are able to build structures perpendicular to the external field. The mixture allows the assembly into two-dimensional networks induced by an one-dimensional field and this effect is of great interest in synthesizing new responsive materials. The formation of dipoles without field was also studied recently [3]. We use Monte-Carlo simulations to study the assembly of such particles and the physical properties of the resulting networks. Further we focus on the influence of macroscopic parameters like concentration and density on these properties.

[1] S. Gangwal, A. Pawar, I. Kretzschmar, and O. D. Velev, Soft Matter 6, 1413 (2010).

[2] H. Schmidle and S. H. L. Klapp, J. Chem. Phys. 134, 114903 (2011).

[3] H. Schmidle, C. K. Hall, O. D. Velev, and S. H. L. Klapp, Soft Matter (2011), accepted.

15 min break

CPP 34.7 Thu 17:00 C 130

Predicting DNA-mediated colloidal interactions with a simple self-consistent mean-field model — •Stefano Angioletti-Uberti, Bortolo Mognetti, Patrick Varilly, and Daan Frenkel — Department of Chemistry, University of Cambridge, Lensfield Road, CB2 1EW Cambridge, UK

We present a general model able to describe with semi-quantitative accuracy the interaction energy between micron-sized DNA coated colloids (DNACCs). The generality of this theory, based on a self-consistent mean-field approach, allows to treat under the same unifying framework arbitrary mixtures of DNACCs functionalized with various types of DNA-based constructs and nucleotides sequences. We compare our theory with full numerical results from Monte Carlo simulations and we discuss in-depth the thermodynamic consistency of our approach, paying attention to highlight the assumptions in our model and possible ways to relax them. It is expected that the present theory will provide a usefull tool for fast, off-the-shelf calculations of DNA-coated colloids interactions.

CPP 34.8 Thu 17:15 C 130

Modeling swimming active droplets — •Maximilian Schmitt and Holger Stark — Institut für Theoretische Physik, TU Berlin

In a recent attempt to build an active microswimmer, a micron-sized droplet of bromine water was placed into a surfactant laden oil medium such that the surfactant molecules spontaneously assemble at the droplet interface [1]. Experiments revealed that due to a bromination reaction of the surfactant (mono-olein), the surface tension locally increases. At the same time these surfactants with a higher surface tension are readily replaced by surfactants from the surrounding oil phase. As a result, a steady gradient of surface tension on the droplet is created. Since an interface with higher surface tension pulls more strongly on a surrounding liquid than one with a lower surface tension, the surface tension gradient on the droplet generates the so-called Marangoni flow.

In order to understand the swimming mechanism, we establish a model based on a free energy functional for the droplet interface. The free energy accounts for the mixing entropy, interactions between the surfactant molecules, and adsorbtion/desorbtion of surfactants from/into the bulk medium. After also taking into account the bromination and the Maranogi flow, we arrive at a reaction-advection diffusion equation on a sphere. Numerical simulations are carried out in order to obtain the flow field at the interface and the swimming trajectory of the droplet.

[1] Shashi Thutupalli *et al* 2011 *New J. Phys.* **13** 073021

CPP 34.9 Thu 17:30 C 130

Self-assembled nematic defect-structures for Janus beads — •Michael Melle[1], Sergej Schlotthauer[1], and Martin Schoen[1,2] — [1]Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany — [2]Department of Chemical and Biomolecular Engineering, North Carolina State University, 911 Partners Way, Raleigh, NC 27695, U.S.A.

We present Monte Carlo simulations of a colloid embedded in a nematic liquid crystal host. Employing different alignment scenarios for the liquid crystal molecules on the surface of the colloid our model is able to reproduce known defect structures of the liquid crystal, such as Saturn ring, surface ring, or Boojum defect to high accuracy and over a wide range of parameters like temperature, pressure or strength of alignment. However, the main focus of this study is on inhomogeneous, spherical colloids such as Janus beads. Despite the large interest that Janus beads have attracted in the last decade, almost no work has been done on the defect structures generated by them. Therefore, we also develop different alignments for different sides of the colloid. We are able to reproduce experimentally known defect structures for Janus beads. In addition, we also predict new topologies. Furthermore, we see transitions between different defect structures induced by a slight decrease of temperature, which is a novel observation as well.

CPP 34.10 Thu 17:45 C 130

Particles as emulsion stabilizers: a simulation study — •Jens Harting[1,2], Stefan Frijters[1], and Florian Günther[1] — [1]Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands — [2]Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany

Emulsions stabilized by particles are ubiquitous in the food and cosmetics industry, but our understanding of the influence of microscopic fluid-particle and particle-particle interactions on the macroscopic rheology is still limited. Modern simulation algorithms based on a multicomponent lattice Boltzmann model to describe the solvents combined with a molecular dynamics solver for the description of the suspended particles allow to tune the particle size, shape, wettability and surface tensions between the fluids. Further, they are ideal candidates to harness the power of today's largest available supercomputers allowing to model small macroscopic systems with microscopic resolution.

We report on the adsorption of spherical or ellipsoidal particles to liquid interfaces and demonstrate the existence of stable and semi-stable equilibrium states. On larger scales, different phases of stabilized emulsions have been found. While Pickering emulsions are already known for more than a century, so-called bicontinuous interfacially jammed emulsion gels (Bijels) where only predicted recently. The particles can fully arrest domain growth and a transition between both phases can be found by tuning the concentration, contact angle, or fluid ratio. Further, by tuning the particle shape additional geometrical degrees of freedom add additional time scales to the arrest of domain growth.

CPP 34.11 Thu 18:00 C 130

Resonances arising from hydrodynamic memory - The Color of Brownian motion — •Sylvia Jeney[1], Matthias Grimm[1], Flavio Mor[1], Laszlo Forro[1], and Thomas Franosch[2] — [1]Laboratory of Physics of Complex Matter, Ecole Polytechnique Fédérale de Lausanne, Switzerland — [2]Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Germany

Observation of the Brownian motion of a small probe interacting with its environment is one of the main strategies to characterize soft matter. Initially, the particle is driven by rapid collisions with the surrounding solvent molecules, referred to as thermal noise. Later, the friction between the particle and the viscous solvent damps its motion. Conventionally, thermal force is taken to be characterized by a Gaussian white noise spectrum. The friction is assumed to be given by the Stokes drag, suggesting that motion is overdamped at long times, when inertia becomes negligible. Here, we measured the noise spectrum of the thermal forces by tracking with high resolution a single micron-sized sphere suspended in a fluid, and confined by a stiff optical trap [1]. Coupling between sphere and fluid gives rise to hydrodynamic memory [2] and a resonance, equivalent to a colored peak in the power spectral density of the sphere*s thermal fluctuations. Our results reveal that motion is not overdamped, even at long times. In view to exploit the particle-fluid-trap system as a nanomechanical resonator, we disentangle the two regimes in which the detected resonance is either sensitive to the fluid properties or to the particles mass. [1] Jeney et al. Nature 2011. [2] Jeney et al. PRL 2008.

CPP 34.12 Thu 18:15 C 130

Magnetic nanorods: A Monte Carlo study — •Carlos E. Alvarez and Sabine H. L. Klapp — Institut für Theoretische Physik, TechnischeUniversität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We perform Monte Carlo simulations of model stiff magnetic nanorods composed of several magnetic hard spheres. We study the thermodynamic properties as well as the structure formation and percolation properties of the system with and without an applied external magnetic field for various densities and temperatures. We measure a critical path approximation for the conductance of the system [1] and observe how it is affected by the length of the rods, the temperature of the system and the presence and strength of an applied external field. We also look at dipolar prolate spheroids [2] as models for magnetic nanorods and compare the results with the multi-sphere rod model.

[1] G. Ambrosetti, C. Grimaldi, I. Balberg, T. Maeder, A. Danani and P. Ryser, *Phys. Rev. B*, **81**, 155434 (2010).

[2] G. J. Zarragoicoechea, J.-J Weis and D. Levesque, *Mol. Phys.*, **74**, 629 (1991).

CPP 34.13 Thu 18:30 C 130

Magnetic particles with shape anisotropy — Sofia Kantorovich[1,2] and •Elena Pyanzina[2] — [1]Institute for Computational Physics, Pfaffenwaldring 27, 70569 Stuttgart, Germany — [2]Ural Federal University, Lenin av 51, 620083, Ekaterinburg, Russia

Anisotropic particles form the cutting edge of dipolar soft matter research as they correspond completely to the idea of fine tuning and designing new materials with controllable properties. In this contribution we present a theoretical study and computer simulations on the ground states, and room temperature behaviour of magnetically capped colloids, magnetic ellipsoids, cylinders and cubes. We analyse in detail how the particle anisotropy can be used in fine-tuning of the properties and macro responses of the systems.

CPP 35: Focus: Rheology I (joint focus with DRG)

Rheology is the science of flow and deformation properties of materials. It covers a vast class of materials from biological cells to synthetic polymers and from food to paint. Only the cooperation of physicists, chemists, engineers and mathematicians allows to handle such a complexity. It is the aim of the focus session to bring scientists from different fields together and allow the exchange of modern rheological methods that have been developed in different areas but can be used on a variety of systems. The first session will have a focus on biological materials and colloids and the second session on polymers. (Organizer: Christian Wagner)

Time: Thursday 15:00–18:45 Location: C 243

Invited Talk CPP 35.1 Thu 15:00 C 243

Motion of microswimmers governed by light in a fluid flow. — •Philippe Peyla, Salima Rafaï, and Xabel Garcia — Grenoble University and CNRS, LIPHY, BP 87 38 402 Saint Martin d'Heres, France

In nature, organisms that can propel themselves in a fluid medium are ubiquitous. While larger organisms, such as fish, use inertia in their motion, microorganisms like spermatozoa, microalgae or bacteria, move at low Reynolds number, where viscous forces dominate over the effects of inertia. A recent and currently unresolved issue involves understanding the hydrodynamics associated with the individual or collective motion of microswimmers through their fluid-mediated interactions. The motion of these micro-organisms is affected by the presence of gradients (chemiotaxis in the presence of chemicals, gyrotaxis in a gravity field, phototaxis under illumination). In this experimental and theoretical work we show how to use the phototaxis properties of some micro-algae to modify and control the flow of a suspension of microswimmers.

CPP 35.2 Thu 15:30 C 243

Active viscosity of bacterial suspensions — •Anke Lindner, Jeremie Gachelin, Helene Berthet, Annie Rousselet, Gaston Mino, and Eric Clement — PMMH-ESPCI, 10, rue Vauquelin, 75231 Paris Cedex 05, France

Active suspensions are fluids laden with self-swimming entities such as bacteria, algae or artificial swimmers. The self-propelled particles inject energy into the suspending fluid, leading to very different properties of active compared to passive suspensions. In particular, it has been predicted theoretically that the viscosity of suspensions of so called pushers can be reduced compared to the viscosity of the suspending fluid.

Pioneering experimental measurements have confirmed that finding, but no bulk rheological experiments at controlled shear rates exist up to date. Here we present experiments measuring the viscosity of a wild type E-Coli suspension. To this purpose, we use a Y shaped microfluidic channel as a rheometer allowing us to resolve small differences between the viscosity of the suspending fluid and the active suspension at low shear rates and with a high resolution. We systematically vary the shear rate and the bacterial density. In this way we show that in a specific range of parameters the viscosity of the active suspension is lower than the viscosity of the suspending fluid. We discuss our results in the perspective of recent theoretical and experimental works .

CPP 35.3 Thu 15:45 C 243

Rheological properties of living and dead microalgae suspensions at various concentrations: the crossover between shear thinning and apparent yield stress behavior — •Antoine Soulies[1], Jack Legrand[1], Jeremy Pruvost[1], Cathy Castelain[2], and Teodor Burghelea[2] — [1]Universite de Nantes, CNRS, GEPEA UMR-CNRS 6144, Bd de l'Universite, CRTT-BP 406, 44602 Saint-Nazaire Cedex, France — [2]Universite de Nantes, CNRS, Laboratoire de Thermocinetique de Nantes, UMR 6607, La Chantrerie, Rue Christian Pauc, B.P. 50609, F-44306 Nantes Cedex 3, France

A systematic study of the rheological properties of solutions of microalgae suspensions (Chlorella) in a wide range of volume fractions is presented. At low volume fractions the suspensions display a Newtonian behavior and the volume fraction dependence of the viscosity can be well described by the Quemada model (Quemada 2006). For intermediate values of the volume fraction a shear thinning behavior is observed and the volume fraction dependence of the viscosity can be described by the Simha model (J. Appl. Phys, 23, 1952). For the largest volume fractions, an apparent yield stress behavior is observed. Increasing and decreasing stress ramps within this range of volume fractions indicate a thixotropic behavior. The rheological data acquired within the high concentration regime bears similarities with the measurements performed by Heymann et al. (Heymann et al. Phys. Rev E 75, 2007) on PMMA suspensions: irreversible flow behavior, dependence of the flow curve on the characteristic time of forcing. Solutions of dead microalgae generally behave similarly to that of living ones.

CPP 35.4 Thu 16:00 C 243

In situ large amplitude oscillatory shear (LAOS) experiments on rod-like viruses and colloidal platelets — •Pavlik Lettinga[1], Peter Holmqvist[1], Simon Rogers[1], Pierre Ballesta[1], Dina Kleshchenok[2], Bernd Struth[3], and Joachim Kohlbrecher[4] — [1]Forschungszentrum Jülich, Jülich,Germany — [2]van 't Hoff Laboratory, Utrecht University, The Netherlands — [3]Desy, Hamburg, Germany — [4]PSI, Villigen, Switserland

Highly anisotropic particles are by nature susceptible to external fields. In particular shear forces can cause a pronounced shear thinning, where a highly viscous unordered system is sheared into a low viscous ordered system. The rheological and structural responses of the system at the onset of shear thinning can be conveniently studied by large amplitude oscillatory shear in combination with in situ scattering techniques. Here we study two systems around the isotropic - nematic: dispersions of rod-like (fd) viruses in combination with time-resolved small-angle neutron scattering and dispersions of gibbsite platelets in combination with time-resolved small-angle X-ray scattering. Viewing the responses as indicating a sequence of physical processes, we identify, for the rod-dispersions, a region of purely elastic response accompanied by an increase in the orientational ordering. By yielding this is followed in sequence by a region of fluid-like behavior at an almost constant ordering. The platelet dispersions display, for a broad range of frequencies, a transition from singlet feature in the scattering at small strain amplitude to a doublet at large strain amplitude. This critical strain for reorienting the platelets is not reflected in the bulk rheology.

CPP 35.5 Thu 16:15 C 243

Nonlinear active micro-rheology of dense colloidal suspensions — •Thomas Voigtmann[1,2,3], Matthias Fuchs[1], Christian Harrer[1], and Manuel Gnann[1] — [1]Fachbereich Physik, Universität Konstanz — [2]Zukunftskolleg, Universität Konstanz — [3]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln

Active microrheology is a powerful tool to probe the local dynamics and rheological properties of a complex material, monitoring the response to external driving applied to a tracer particle. Especially the nonlinear-response regime reveals a wealth of information, but is less obvious to analyze than the linear response. We present recent advances in the framework of mode-coupling theory and the integration-through-transients formalism for force-driven microrheology, applying a constant force to a probe embedded in a dense, glass-forming colloidal suspension. A typical signature seen in experiment and computer simulation is a pronounced force-thinning, i.e., a strong reduction of the local friction at forces large compared to those induced by thermal fluctuations. We discuss this nonlinear effect in terms of a delocalization transition for the probe particle. We also address the limit of strong driving, where a non-trivial high-force plateau in the probe's friction coefficient is observed. Connections of these microscopic quantities to macroscopic rheological properties of the host liquid, and possible universalities among different system classes will also be discussed.

[1] I. Gazuz *et al.*, Phys. Rev. Lett. **102**, 248302 (2009).

[2] M. V. Gnann *et al.*, Soft Matter **7**, 1390 (2011).

CPP 35.6 Thu 16:30 C 243

Non-equilibrium Forces between Dragged Ultrasoft Colloids — •Sunil P. Singh, Roland G. Winkler, and Gerhard Gompper — Institute of Complex Systems and Institute for Advanced Simulation,Forschungszentrum Juelich, 52425 Juelich, Germany

Ultrasoft colloids, such as, star polymers, in a suspension strongly interacted with each other under non-equilibrium conditions. Contact of two soft colloidal macromolecules may lead to large conformational changes and significant frictional forces, which determine the macroscopic rheological properties of the fluid. To arrive at an understanding of the non-equilibrium dynamical properties of ultrasoft colloids, we numerically investigate the deformation as well as dynamic frictional forces when two star polymers dragged past each other at constant velocity. We apply a hybrid simulation approach combining with multiparticle collision dynamics method for the solvent, with molecular dynamics simulations for the star polymers. We compute the dynamical frictional forces as function of the drag velocity. At vanishing relative velocity, the equilibrium repulsive force-distance curve is obtained. With increasing drag velocity, this behavior changes and we find an apparent attractive force for departing stars along the dragging direction. The close encounter of ultrasoft colloids leads to significant deformations. This behavior can be traced back to the retardation of polymer relaxation and symmetry breaking of the polymer conformations relative to the mid-plane between the polymer centers.

15 min break

CPP 35.7 Thu 17:00 C 243

Direct observation of translation and rotation of aggregated colloids under mechanical load — •Jennifer Wenzl, Marcel Roth, and Günter K. Auernhammer — Max Planck Institute for Polymer Research, Mainz, Germany

The correlation between single particle interactions and meso- or macroscopic behavior of colloidal and granular matter is still not well understood. The challenge in 3D systems is to measure deformation, translation, and especially rotation of particles and agglomerates. Using confocal microscopy to obtain time resolved 3D imaging we track the particle positions. Introducing internal optical anisotropy allows us additionally to measure the rotation of spherical particles without changing their interaction. From the measured data we determine for every labeled particle both rotation angles. Combining mechanical load with simultaneous 3D microscopic imaging we explore the correlation between local structure, translation and rotation of the particles and the overall deformation of the system.

CPP 35.8 Thu 17:15 C 243

Transient rheology of concentrated suspensions — •Miriam Siebenbürger[1], Thomas Voigtmann[2,3,4], Christian Amann[2], Matthias Fuchs[2], and Matthias Ballauff[1] — [1]Institut für Weiche Materie und Funktionale Materialien, Helmholtz Zentrum Berlin für Materialien und Energie, Berlin, Deutschland — [2]Fachbereich Physik, Universität Konstanz, Konstanz, Deutschland — [3]Zukunftskolleg, Universität Konstanz, Konstanz, Germany — [4]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, Deutschland

Suspensions of sherical thermosensitive core-shell colloids are excellent model system for the study of the fluid to glass transition. In the last years the phase behavior, the linear [1] and nonlinear [2] viscoelastic properties as well as the rheological properties in stationary flow could be described in detail with the Mode Coupling Theory (MCT). Here we report on the transient rheology of these suspensions: i) For the start-up of shear aging-dependent overshoot phenomena are observed experimentally. The overshoot was also found by simulations [3] and can be described by a new schematic MCT-model. ii) The stress relaxation after switching off steady shear was found to be sensitive for the onset of the glassy state. iii) Finally, we present a systematic investigation of the creep behavior of the suspension in the glassy state.

References:

[1] M. Siebenbürger et al., J. Rheol. 53, 707 (2009).

[2] J. M. Brader et al., Phys. Rev. E 82, 061401 (2010).

[3] J. Zausch et al., J. Phys. Condens. Mat. 20, 404210 (2008).

CPP 35.9 Thu 17:30 C 243

Rheological Distinction between Gels and Soft Glasses during Critical Slowdown of their Relaxation Dynamics — •Horst Henning Winter — National Science Foundation, Arlington VA, USA, and University of Massachusetts Amherst MA, USA

Gels and soft glasses are difficult to distinguish rheologically because both show a critical slow down in the approach of the liquid-to-solid transition. The dynamics is dominated by the diverging, longest relaxation time, tau,max, which assumes a noticeably large values and is hard to measure because of that. The difference between gels and soft glasses, however, becomes apparent in the distinct pattern of the relaxation spectrum of the critical slowdown. While the long-time component of the relaxation time spectrum follows a powerlaw in relaxation time for both, log H~n log tau, their powerlaw exponent n is of different sign: negative n for the critical gel(material at the gel point) (Chambon et al. Polym Bull 13:499,1885; Winter et al. J Rheology 30:367, 1986; Chambon et al. J Rheol 31:683,1987) and positive n for the soft glass (Siebenbürger et al. J Rheology 53:707,2009; Winter et al. Rheol Acta 48:747, 2009).The powerlaw spectrum is cut off by the diverging, longest relaxation time (called alpha relaxation time for the soft glass, tau,max=tau,alpha) in the approach of the liquid-to-solid transition. In summary, patterns in the relaxation data provide a clear distinction between these two classes of materials.

CPP 35.10 Thu 17:45 C 243

Thermal convection in a nonlinear non-Newtonian magnetic fluid — David Laroze[1,2] and •Harald Pleiner[1] — [1]Max Planck Institute for Polymer Research, Mainz — [2]Instituto de Alto Investigacion, Universidad de Tarapaca, Arica, Chile

We report theoretical and numerical results on the convection of a magnetic fluid in a viscoelastic carrier liquid. The non-Newtonian material properties are taken care of by a general hydrodynamic nonlinear viscoelastic model [1] that contains, but is more general than the standard Oldroyd and Giesekus phenomenological rheological equation for the stress tensor. We calculate the linear threshold for both idealized and rigid boundary conditions and make the comparison with the linear Oldroyd magnetic fluid [2]. In order to explore the nonlinear behavior we perform a truncated Galerkin expansion obtaining a generalized Lorenz system. We find numerically the system's stationary, periodic and chaotic regimes. Finally, we give a phase diagram depicting the various types of dynamical behavior as a function of the Rayleigh number and the viscoelastic material parameters.

[1] H. Pleiner, M. Liu, H.R. Brand, Rheol. Acta. 43, 502 (2004).

[2] L.M. Pérez, J. Bragard, D. Laroze, J. Martinez-Mardones, H. Pleiner, J. Mag. Mag. Mat. 323, 691 (2011).

CPP 35.11 Thu 18:00 C 243

Two-dimensional microrheology of freely-suspended liquid crystal films — •Alexey Eremin, Sebastian Baumgarten, Sarah Dölle, and Ralf Stannarius — Otto-von-Guericke Universität, IEP/ANP, 39106 Magdeburg

It is well known that the hydrodynamic modeling of flow in two dimensional (2D) systems poses special problems that can be more complex than the three-dimensional counterparts, e.g. Stokes* paradox for the motion of disks in a 2D liquid membrane. Flow phenomena in restricted geometries have been intensively studied in the last years with implications to different physical, chemical and biological systems. Those studies usually employ indirect measurements of the inclusion mobilities, for the lack of a convenient 2D model system. On the other hand, smectic liquid crystals can form freely-suspended films of uniform structure and thickness, making them ideal systems for studies of

2D hydrodynamics. We have measured particle mobility and shear viscosity by direct observation of the gravitational drift of silica spheres, droplets and smectic islands included in these fluid membranes. In thick films, we observe a hydrodynamic regime dominated by lateral confinement, with the mobility of the inclusion determined predominantly by coupling of the fluid flow to the fixed boundaries of the film. In thin films, the mobility of inclusions is governed primarily by coupling of the film fluid to the surrounding air, as predicted by Saffman-Delbrück theory. A crossover between both regimes is observed.

CPP 35.12 Thu 18:15 C 243

Ermittlung der Axialkraft während der kapillaren Verjüngung von Fluidfäden (CaBER- Methode) — •Dirk Sachsenheimer, Bernhard Hochstein, Hans Buggisch und Norbert Willenbacher — Karlsruher Institut für Technologie, Institut für Mechanische Verfahrenstechnik und Mechanik, Karlsruhe, Deutschland

Die Capillary Breakup Extensional Rheometry (CaBER) ist eine vielseitig anwendbare Methode zur Charakterisierung der Dehnviskosität niedrigviskoser, komplexer Fluide. Im Gegensatz zu anderen Messverfahren können sehr große, praxisrelevante Gesamtdehnungen erreicht werden. Die Bestimmung der Dehnviskosität ist jedoch eingeschränkt, weil die Zugkraft am Fluidfaden bisher nicht erfasst wird. Wir der Fluidfaden im Gegensatz zu dem herkömmlichen CaBER-Experiment nicht senkrecht, sondern horizontal verstreckt, so ermöglicht die Durchbiegung des Fadens die Berechnung der Axialkraft. Mit Hilfe dieser neuartigen Versuchsführung kann experimentell gezeigt werden, dass die Annahme der verschwindenden axiale Normalspannung für viskoelastische Fluide, die im CaBER-Experiment zylindrische, sowie mit der Zeit exponentiell abfallende Fäden bilden, im Rahmen der Messgenauigkeit gerechtfertigt ist. Im Gegensatz hierzu zeigen Newtonsche Fluide eine stärkere Durchbiegung. Diese ist auf eine negative axiale Normalspannung zurückzuführen. Mittels der experimentell bestimmten Kraft, sowie der zeitlichen Abnahme des Fadendurchmessers kann die wahre Dehnviskosität berechnet werden. Für Newtonsche Fluide ist diese erwartungsgemäß das Dreifache der Scherviskosität. Für viskoelastische Fluide wird ein deutlich größeres Verhältnis ermittelt.

CPP 35.13 Thu 18:30 C 243

Rheology of human blood plasma: Viscoelastic versus Newtonian behaviour — •Matthias Brust[1], Christof Schaefer[1], Roland Doerr[1], Paulo Arratia[2], and Christian Wagner[1] — [1]Experimentalphysik, Universität des Saarlandes, Saarbrücken, Germany — [2]Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia, USA

We investigated the rheological characteristics of human blood plasma using three different flow experiments, namely the capillary breakup extensional rheometer (CaBER), a commercial rotational shear rheometer, and the shear flow in a contraction microfluidics. While the shear experiments showed a Newtonian behaviour, we found a viscoelastic behaviour of blood plasma in the pure extensional experiment. Comparing the results with those of a low concentrated polymeric fluid (PEO) with matchable rheometric characteristics in terms of elongational relaxation time and shear viscosity showed a consistent picture in all experiments. The results are discussed with regard to their relevance concerning venous blood flow in the human body.

CPP 36: Wetting, Micro and nanofluidics I

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

Topical Talk CPP 36.1 Thu 15:00 C 264

From superhydrophobic to superamphiphobic coatings: How to tune wetting — •Doris Vollmer, Xu Deng, Lena Mammen, Periklis Papadopoulos, and Hans-Jürgen Butt — MPI for Polymer Research, Mainz, Germany

Many surfaces in nature are superhydrophobic, for example lotus leaves. Microscopic pockets of air are trapped beneath the water drops. This composite interface leads to an increase in the macroscopic contact angle and a reduced contact angle hysteresis [1]. However, the addition of an organic liquid such as alcohol or oil, decreases the interfacial tension sufficiently to induce homogeneous wetting. Drops, initially resting on air pockets, pass the transition to complete wetting (Wenzel state). Coatings that are simultaneously superhydrophobic and superoleophobic, i.e. superamphiphobic, are rare. For superamphiphobicity, surface roughness, low surface energy and topography are essential. We designed a transparent superamphiphobic using candle soot as a template [2]. Soot consists of a fractal-like assembly of nano-spheres. Convex small-scale roughness can provide a sufficient energy barrier against wetting, even if the Wenzel state is the thermodynamic equilibrium state. Finally, we discuss the coating resistance against drop impact.

[1] D'Acunzi, L. Mammen, M. Singh, X. Deng, M. Roth, G.K. Auernhammer, H.-J. Butt, and D. Vollmer, Faraday Discus. 146 (2010), 35.

[2] X. Deng, L. Mammen, H.-J. Butt, and D. Vollmer; Transformation of black candle soot into a transparent robust superamphiphobic coating, Science in press.

CPP 36.2 Thu 15:30 C 264

Influence of surfactant concentration and transport on forced dynamic wetting — •Daniela Fell[1,2], Ngamjarassrivichai Pawanrat[1,3], Manos Anyfantakis[1], Elmar Bonaccurso[2], Hans-Jürgen Butt[1], and Günter K. Auernhammer[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Center of Smart Interfaces, Darmstadt, Germany — [3]Chulalongkorn University, Bangkok, Thailand

We study the influence of surfactants as well as their local and nonlocal transport processes on dynamic contact angles in a rotating drum setup. Therefore contact angles of surfactant solutions at concentrations well below the critical micelle concentration (cmc) are measured as a function of wetting/dewetting velocity. Surface transport of surfactant is hindered by the axis holding the cylinder. Changing the filling height from half filled to slightly below or above the axis removes this hindrance. For blocking surface as well as bulk transport an additional metallic barrier is added to a half filled bath.

With increasing surfactant concentration the receding contact angle decreased. Stronger surfactants (low cmc) show a larger decrease of the contact angle than weaker ones. Additionally, at a constant concentration the receding contact angle decreased when increasing the hindrance to surfactant transport. Dynamic contact angles are therefore not only influenced by short-range effects like Marangoni stresses, but also by long-range transport processes like diffusion and advection between regions close to the advancing and receding contact lines.

CPP 36.3 Thu 15:45 C 264

Dynamics of Wet Granulates under Shear Deformation — •Somnath Karmakar[1], Marc Schaber[1], Marco Di Michiel[2], Mario Scheel[2], and Ralf Seemann[1,3] — [1]Saarland University, Saarbrücken, Germany — [2]ESRF, Grenoble, France — [3]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Adding liquid to dry granular matter typically leads to stiffening of the granulate which arises due the formation of wet contacts between individual granules by the virtue of capillary forces. We study the mechanical properties of wet granulates which are composed of spherical glass or basalt beads. The glass is almost perfectly wetted by water whereas the basalt beads have a rather large contact angle with water. Our main focus is on the yield strength which is measured using a particularly designed shear cell which allows to vary shear speed, shear amplitude and absolute pressure. Due to the different wettability, the yield strength of glass granulates depend on the applied shear rate whereas for non-wetting basalt granules, the yield strength is independent of the applied shear rate. Surprisingly, for large absolute pressure, the stiffening of a wet granulate might be inversed and the liquid might rather act as a 'lubricant' lowering the yield strength with respect to dry granulates. With time resolved X-ray tomography, we could shed some light on the peculiar mechanical properties of wet granulates and could identify a liquid exchange process occurring between the individual liquid morphologies which depends on the wettability of wet granular systems.

CPP 36.4 Thu 16:00 C 264

Liquid transport in wet granular packings — •Ciro Semprebon, Stephan Herminghaus, and Martin Brinkmann — Max

Plank Institute for Dynamic and Self Organization, Goettingen

Liquid transport in a static pile of spherical beads can proceed through the formation of a thin wetting film on the surface or through the vapor phase. At sufficiently high surface liquid coverage a wetting film can be formed that percolates through the surface roughness. Assuming a constant effective mobility of this film and stationary flow conditions the local pressure in the film satisfies Laplace's equation with Dirichlet boundary conditions given by the Laplace pressure on the contact line of the bridges. The conductance of the film on a spherical surface in the presence of two bridges can be solved exactly by conformal mapping. Employing a perturbative method we arrive at a simplified model to calculate the matrix elements of the complete conductance matrix for arbitrary bridge configurations. Comparison to finite element methods shows that this approximation is sufficiently precise under certain conditions. The simplified model can be implemented in coarse grained numerical simulations aiming at the liquid transport through large static packings of spherical beads at different liquid saturations.

CPP 36.5 Thu 16:15 C 264

Pore-scale dynamics of multiphase fluid flow through porous media using synchrotron X-ray tomography — •Kamaljit Singh[1,2], Hagen Scholl[3], Marco Di Michiel[1], Mario Scheel[1], Stephan Herminghaus[2], and Ralf Seemann[2,3] — [1]ESRF, Grenoble, France — [2]MPI-DS, Goettingen, Germany — [3]Saarland University, Saarbruecken, Germany

The dynamic behavior of water-oil fronts during a water flood into an initially oil filled porous medium was investigated using ultrafast X-ray tomography at the European Synchrotron Radiation Facility. This type of multiphase flow is similar to a situation which can be found for oil recovery and soil decontamination. We investigated the effect of wettability, flow velocity, porosity and gravity. The findings reveal that the water-oil front is more compact in basalt beads, whereas the front in glass beads progresses in elongated fingers. The fingering in the glass beads results in a higher final residual oil saturation due to bypassing of several oil-filled pores. Secondly, a significant oil movement was observed behind the main front in the case of basalt beads, therefore sweeping the rest of the oil resulting in less trapping after a complete water flood. We further analyzed the time-series of tomograms to identify preferential pathways during forced-imbibition. These flow paths are overlain by corresponding pore-throat network to investigate the properties of pores and throats allowing water-oil interfaces to migrate. From this analysis, it seems that capillary forces dominate the flow behavior instead of hydraulic resistance. Finally, the velocity does not seem to play a significant role in water-oil front behavior.

CPP 36.6 Thu 16:30 C 264

Dielectric Capillary Rise in Mesoporous Vycor-Glass — •Beatrice Hallouet, Erika Robert, Patrick Huber, and Rolf Pelster — FR 7.2 Experimentalphysik, Universität des Saarlandes, Campus E26, 66123 Saarbrücken

We present a new method to follow the capillary rise of liquids in mesoporous samples by means of dielectric spectroscopy. The mesoporous material is Vycor®, a 3D network with a mean pore radius of about 4 nm and a porosity of about 30 %. The liquids are 1-alcohols (hexanol up to undecanol) which are carbons-chains molecules with one polar group. By measuring the time dependence of the permittivity, we are able to show that the capillary rise follows the so-called Lucas-Washburn law $h(t) = c_h\sqrt{t}$, where c_h depends on fluid parameters (viscosity, surface tension) and matrix parameters (porosity, radius ...). The combination of dielectric and gravimetric measurements allows us to evaluate quantities like the initial porosity or the hydrodynamic radius. We discuss the influence of humidity, i.e. of adsorbed water layers on the pore walls. The flow of all alcohols seems to be characterized by the same hydrodynamic radius but the contact angle may vary as a function of the chain length.

15 min break

CPP 36.7 Thu 17:00 C 264

Imaging of wetting dynamics of a molecularly thin fluid film in a soft graphene-mica slit pore — •Nikolai Severin, Philipp Lange, Igor M. Sokolov, and Jürgen P. Rabe — Department of Physics, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

The behavior of water and other molecular liquids confined to the nanoscale is of fundamental importance, e.g., in biology, material science, nanofluidics and tribology. Direct microscopic imaging of wetting dynamics in sub-nanometer pores is however challenging. We demonstrate high resolution imaging of a molecularly thin water film wetting the interface between mica and graphene. Ambient humidity allows to control the wetting and dewetting of the film. We follow these processes in space and time using scanning force microscopy imaging of the graphene conforming to the film. At sufficiently high humidity a continuous molecularly thin water film wets the interface between the graphene and mica. At lower humidities the film dewets with fractal depressions exhibiting dimensions around 1.7 and depths comparable to the size of a water molecule. The soft graphene cover offers a previously unexplored semi-hydrophilic slit pore of self-adjustable size, which enables high resolution imaging of confined molecularly thin fluid films. Moreover, the self-adjusting slit pore geometry implies prospects to experiment with other liquids and liquid mixtures with molecules of variable sizes. The soft electrically conducting cover offers interesting opportunities for the fabrication of novel nano-fluidic devices including an electrically driven pump.

CPP 36.8 Thu 17:15 C 264

Wetting and adsorption properties of monolayer interfaces — •Jens Smiatek[1], Hendrik Wagner[2], Armido Studer[2], and Andreas Heuer[1] — [1]Institut für Physikalische Chemie, WWU Münster, D-48149 Münster, Germany — [2]Institut für Organische Chemie, WWU Münster, D-48149 Münster, Germany

We present the results of mesoscopic Dissipative Particle Dynamics (DPD) simulations concerning monolayers with varying length in contact with an explicit solvent. Our results indicate different solvent interface concentrations for varying monolayer thicknesses. Additionally we have calculated the free binding energy for a test particle. Our results demonstrate that the test particle is stronger adsorped at thinner monolayers due to a decreased solvent content and a higher monomer density at the interfacial region. The numerical findings are in good agreement with experimental observations.

CPP 36.9 Thu 17:30 C 264

Parameter passing between Molecular Dynamics and thin film hydrodynamics — •Nikita Tretyakov[1], Marcus Müller[1], Desislava Todorova[2], and Uwe Thiele[2] — [1]Institut für Theoretische Physik, Georg-August-Universität, Göttingen, Germany — [2]Department of Mathematical Sciences, Loughborough University, Loughborough, UK

First, we study the wetting properties of coarse-grained polymer liquids by Molecular Dynamics (MD) simulation. The system consist of a LJ-polymer liquid on a fcc lattice substrate. The temperature is controlled by a DPD thermostat, which locally conserves momentum. The values of the contact angle are dictated by the strength of the substrate-liquid interaction.

At small thicknesses of a polymer film the interaction of the substrate-liquid and liquid-vapor interfaces can be expressed by the Derjaguin (or disjoining) pressure. In the MD simulations we measure the Derjaguin pressure and the surface tension through the anisotropy of the pressure tensor using a slab geometry. The Derjaguin pressure and surface tension are then employed to predict the shape of droplets using two continuum models that correspond to the static limit of a hydrodynamic thin film equation in full-curvature and long-wave formulation, respectively. The results are compared to the averaged profiles in particle simulation.

We acknowledge support by the EU (PITN-GA-2008-214919).

CPP 36.10 Thu 17:45 C 264

The influence of nano-roughness on solid-liquid surface free energies. A molecular dynamics simulations contribution. — •Frédéric Leroy — TU-Darmstadt, Darmstadt, Germany

We address the question of the determination of the surface free energies of rugged solid-liquid interfaces. We aim to describe interfaces whose roughness dimension is of the order of 1-10 nanometers. Although such surfaces are ubiquitous, the way nanostructures influence the solid-liquid surface free energy remains largely unexplored. This is mainly due to the impossibility to carry out direct measurements of this quantity. Its estimation relies on droplets contact angles measurements and on the use of equations to connect surface free energies and contact angles. There is experimental evidence that this task is not always straightforward to be performed. It is also legitimate to wonder whether continuum equations have the ability to describe situations where molecular details may matter.

We introduce a thermodynamic integration algorithm to determine the surface free energy of smooth and rugged interfacial systems. We perform molecular dynamics calculations dealing with water in collapsed wetting states on model rugged graphite-based surfaces simultaneously exhibiting roughness and chemical heterogeneity. We show that the related continuum theory is able to predict the nanometer scale results under the condition that water does not experience too strong confinement. Our results also evidences that the origin of surface free energy, at least in the case of water on non-polar attractive substrates, is to be found in the very few first layers of adsorbed water.

CPP 36.11 Thu 18:00 C 264

Wetting and prewetting in electrolyte solutions — •Ingrid Ibagon, Markus Bier, and S. Dietrich — Max-Planck-Institut IS, Stuttgart, Germany

We investigate the wetting of a charged substrate by an electrolyte solution by means of classical density functional theory applied to a lattice model for an ionic fluid. Our lattice model consists of three species (solvent, anions and cations) that occupy the sites of a uniform lattice filling the half-space z>0. The three species have an attractive nearest-neighbor interaction. Moreover ions interact via Coulomb force and all three species interact with the substrate via an attractive external potential. The surface charge density and the ionic concentration are found to have an impact on the wetting behavior, in particular the influence on the wetting temperature and the prewetting transition are studied.

CPP 36.12 Thu 18:15 C 264

Dynamics of small droplets on solid surfaces — •Nasrollah Moradi[1], Fathollah Varnik[1,2], and Ingo Steinbach[1] — [1]ICAMS, Ruhr Universität Bochum — [2]Max-Planck Institut für Eisenforschung,

The behavior of individual microdrops on solid surfaces is very important in many practical processes [1,2]. Despite of its importance, many aspects of this behavior, however, are still not well understood. Here, we address some of these aspects. The main focus is on the behavior of small drops on a super hydrophobic surface with a gradient of roughness; the effect of a step wise change in the pillar density on the dynamics of drops is investigated via lattice Boltzmann (LB) simulations [3], and the dependence of the drop velocity on the surface tension and the gradient of pillar density is analytically modeled [4]. In addition to the case of drops on a gradient of roughness, based on a detailed LB survey of the local viscous dissipation inside sliding droplets on flat substrates, we model the dependence of the drop velocity on the equilibrium contact angle [5]. Finally, we study the behavior of droplets at situations in which the size of a droplet is comparable to the roughness scale of the solid substrate using LB simulations. In this case, possible morphologies and a so-called re-entrant transition are studied [6].

1- P. G. de Gennes, Rev. Mod. Phys. 57, 827 (1985) 2- C. Dorrer and J.Rühe, Soft Matter 5, 51 (2009) 3- M. R. Swift, W. R. Osborn and J. M. Yeomans, PRL 75, 830 (1995) 4- N. Moradi, F. Varnik and I. Steinbach, EPL 89, 22006 (2010) 5- N. Moradi, F. Varnik and I. Steinbach, EPL 95, 44003 (2011) 6- N. Moradi, F. Varnik and I. Steinbach, MSMSE 19, 45005 (2011)

CPP 36.13 Thu 18:30 C 264

Wetting of droplet ensembles on solid substrates — •Marouen Ben Said[1,2], Britta Nestler[1,2], Harald Garcke[3], and Michael Selzer[1,2] — [1]Institute of Materials and Processes, University of Applied Sciences, Karlsruhe, Germany — [2]Institute of Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Faculty of Mathematics, University of Regensburg, Regensburg, Germany

We present a phase field model for multi-phase systems with preserved volume fractions and an accurate boundary condition to simulate wetting behaviors of droplet ensembles on solid substrates. The formulation of the boundary condition at the substrate surface ensures the correct macroscopic contact angles according to Young's law. The approach is related to the minimization of free energy of the system. Furthermore, we use the energy formulation proposed by Nestler et al. [1] with an additional substrate energy term describing the interactions between the solid- and the different liquid phases. We show 2D and 3D simulations of liquid droplet ensembles on flat and structured solid walls and discuss the results.

[1] Britta Nestler, Frank Wendler, Michael Selzer, Björn Stinner, and Harald Garcke. Phase field model for multi-phase systems with preserved volume fractions. *Phys. Rev. E*, 78(1):011604, Jul 2008.

CPP 37: Poster: Rheology (joint focus with DRG)

Time: Thursday 18:45–19:45 Location: Poster A

CPP 37.1 Thu 18:45 Poster A

Active fluids in Taylor Couette Systems — •Matthias Mussler, Albrecht Ott, and Christian Wagner — Universität des Saarlandes, Saarbrücken

The behavior of active fluids is poorly understood. Here we study experimentally the hydrodynamic behavior of active polar gels using the methods of rheology and particle tracking (PT) in a Taylor-Couette Geometry. Taylor-Couette hydrodynamics are well-understood for passive fluids, such as polymer solutions. Active fluids are expected to show deviations from passive behavior. Micro-swimmer suspensions of Chlamydomonas Reinhardtii are suitable model systems for studying active fluids. The presence of active swimmers increased the viscosity and is not yet understood. Experiments using the methods of Rheology and Optical Tweezers are performed to study these systems.

CPP 37.2 Thu 18:45 Poster A

The reversibility of modifications created by processing linear and long chain branched polypropylene melts — •Bernadette Duscher[1,2], Alois Schausberger[2], and Wolfgang Stadlbauer[1] — [1]Transfercenter für Kunststofftechnik GmbH, Franz-Fritsch Str. 11, A-4600 Wels — [2]Johannes Kepler University, Altenberger Str. 69, A-4040 Linz

The rheological properties of long chain branched polypropylene (LCB-PP) and of its blends with linear PP (L-PP) are strongly affected by processing time, temperature, machining method and even screw configuration. The resultant modification and its reversibility are investigated by means of rheological experiments in shear and elongation. In addition, the flow activation energies (E_a) of process-modified samples are determined in order to describe the entanglement state.

Three different processing methods (measuring mixer, twin-screw extruder with varying screw set-ups) and varying processing parameters have been used. The reduction of dynamic moduli and E_a depends on the operational demands the polymer blend has passed. By dissolving process-modified samples, an equilibrium state is created and the activation energies as well as the rheological properties of the blends are determined. The dynamic moduli do not recover totally but superimpose in a limit function. However, after dissolving E_a of the samples equal those of neat, dissolved and untreated samples. By determining strain hardening behavior, it is shown that the smaller the strain rates are, the higher the difference between the process-modified samples and its dissolved equivalents is.

CPP 37.3 Thu 18:45 Poster A

Complex rheological behavior of epoxy resin based nanocomposites — •Matthieu Thomassey, Jörg Baller, Jan-Kristian Krüger, and Roland Sanctuary — Laboratory of Physics of Condensed Matter and Advanced Materials, University of Luxembourg, 162A, Avenue de la Faïencerie, L-1511 Luxembourg

Rheology is a well-suited tool to reveal flow-induced structural changes in complex soft matter systems. The knowledge of these structural changes is essential to ensure an efficient processing of numerous composites materials. Furthermore it is highly interesting with regards to the fundamental understanding of the mechanisms underlying the structural formation. This contribution presents a detailed rheological study of an oligomer epoxy resin (diglycidylether of bisphenol A) filled either with hydrophilic alumina or hydrophobic silica nanoparticles. For both systems steady-shear viscosity measurements reveal shear-thinning and subsequently shear-thickening behavior when the shear rate increases. Despite similar flow behaviors of both nanocomposites their transient responses at given shear rates are different. Results are discussed in terms of geometry of nanoparticles, particle-particle interactions and interactions between nanoparticles and matrix molecules.

CPP 37.4 Thu 18:45 Poster A

Gap dependence of the trim distance in parallel plate rheometry — •Roman Sebastian Rittberger[1,2] and Gerhard Eder[2] — [1]Transfercenter für Kunststofftechnik GmbH, Wels, Österreich — [2]Institute of Polymer Science, Johannes Kepler Universität, Linz, Österreich

Calculations in parallel plate rheometry rely on cylindrical sample shapes. However, trimming excessive material after sample loading often leads to a slightly dinted rim. Consequently the gap is lowered additionally by the trim distance δ to achieve cylindrical sample geometry. Thus gap dependence of the trim distance δ for a given measurement geometry and material has to be known a priori.

For this investigation polymer samples were melted in the rheometer and the gap was set to trim position H_T. After thermal equilibration excessive melt was removed with an applicator and the samples were quenched to solidify for following weighing. The trim distance is modeled by approximating the rim geometry as parabola and assuming the depth of dint $\Delta r = \Delta r^* H_T$. The model also accounts for potential gap errors. Doing regression analysis on a series of trim positions gives the material specific constant Δr^* and the gap error of the measuring system.

The dependence of the trim distance δ on the trim position H_T was found to be quadratic (higher terms can be neglected). Plotting δ/H_T versus H_T/R leads to a unified representation, which can be deployed for plates with arbitrary radii. The only parameter left is the constant Δr^*, solely depending on the materials properties.

CPP 37.5 Thu 18:45 Poster A

Following UV Induced Chemical Reactions with Rheometry and Simultaneous FTIR-Spectroscopy — •Jan Philip Plog[1], Veit Zschuppe[1], and Manfred Feustel[2] — [1]ThermoFisher Scientific, Dieselstraße 4, 76227 Karlsruhe, Germany — [2]Resultec, Gartenstraße 23, 89171 Illerkirchberg, Germany

In this article a new and unique combination of a rheometer and an FTIR-spectrometer is presented. The so-called Rheonaut module allows the coupling of the Thermo Scientific HAAKE MARS rheometer platform with an FTIR-spectrometer. With this set-up, samples can be characterized rheologically using cone/plate- or plate/plate-geometries while IR-spectra are being recorded simultaneously. To test this new concept, UV induced polymerization and cross-linking reactions have been followed with the combination of HAAKE MARS and the Rheonaut module. Depending on the chemical nature of the components involved, the disappearance of the starting materials reactive group and/or the appearance of chemical groups, which are characteristic for the product can be seen and correlated with the development of the mechanical properties. Details of this unique instrument set-up as well as selected results will be presented.

CPP 37.6 Thu 18:45 Poster A

Decay of elastic turbulence in a von Karman swirling flow — •Christof Schäfer[1], Teodor Burghelea[2], and Christian Wagner[1] — [1]Experimental Physics, Saarland University, 66123 Saarbrücken, Germany — [2]Laboratoire de Thermocinétique, University of Nantes, Nantes 44306, France

We present results of the experimental study of the decay of elastic turbulence in a von Karman swirling flow. We characterize various decay regimes by combined measurements of the integral power injected into the system and local measurements of the velocity gradients as a function of the initial Weissenberg number. Following relevant literature [1] a detailed description of the time evolution of the decaying flow structures is given. The characteristic decay time scales of the locally measured velocity gradients in both the bulk and in the elastic boundary layer of the flow is compared to the characteristic decay times of the integral power, the Eulerian correlation time of velocity fields and the largest relaxation time of the polymer solution. Based on these results, the possibility of exciting nonlinearly unstable states from an initially linearly stable base state is discussed.

[1] T. Burghelea, E. Segre, and V. Steinberg, "Elastic turbulence in a von Karman swirling flow between disks", Phys. Fluids 19, 053104 (2007)

CPP 37.7 Thu 18:45 Poster A

dynamics of thermosensitive core-shell dumbbell-shaped microgels — •Fangfang Chu, Miriam Siebenbürger, Nils Heptner, Joachim Dzubiella, Yan Lu, and Matthias Ballauff — Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 14109 Berlin, Germany

We present a study of the dynamics of dumbbell-shaped microgels. The thermosensitive dumbbell-shaped microgel latices consist of a dumbbell-shaped polystyrene-core and a themosensitive shell of cross-linked poly(N-isopropylacrylamide). These colloidal particles could be synthesized with an uniform size and morphology. The aspect ratio L*, which is defined as the ratio of the center to center distance L and the diameter D, was L*~0.24. Oscillatory experiments in the linear viscoelastic regime and flow curves in the steady sheared state were performed to investigate the phase diagram and the dynamics of concentrated dumbbell suspensions at various volume fractions and aspect ratios. The formation of a plastic crystal phase for higher volume fractions was found which was predicted by simulations [1,2,3]. For the higher volume fractions a glassy like behavior is found.

References 1. C. Vega, P. A. Monson, J. Chem . Phys. 1992, 97, 8543 2. C. Vega, P. A. Monson, J. Chem . Phys. 1997, 107, 2696 3.J. J. Crassous, M. Siebenburger, M. Ballauff, M. Drechsler, D. Hajnal, O. Henrich, M. Fuchs, J. Chem . Phys. 2008, 128, 9606

CPP 37.8 Thu 18:45 Poster A

Unsteady low Reynolds pipe number flows of a Carbopol solution: why the simplest flow problems still remain elusive? — Antoine Poumaere[1], Miguel Moyers-Gonzales[2], •Cathy Castelain[1], and Teodor Burghelea[1] — [1]Universite de Nantes, CNRS, Laboratoire de Thermocinetique de Nantes, UMR 6607, La Chantrerie, Rue Christian Pauc, B.P. 50609, F-44306 Nantes Cedex 3, France — [2]Department of Mathematics and Statistics, University of Canterbury, Private Bag 4800, Christchurch 8140, New Zealand

Carbopol solutions are often referred to as non-thixotropic "model yield stress fluids". It has been only recently shown that this picture does not suffice to tackle simple flow problems, particularly close to yield point (Putz et al., Phys. Fluids 20(3), 2008). The present study focuses on a equally simple flow configuration: a low Reynolds number unsteady pipe flow. Measurements of the unsteady velocity fields allow time-dependent measurements of the mean flow velocity, width of the viscoplastic plug, slip velocity and wall velocity gradients. The dependence of each of these quantities on the applied pressure drop reveals three distinct regimes: a solid regime corresponding to pressure drops significantly below the yield limit, a solid-fluid flow regime corresponding to intermediate flow regimes and a fluid regime far beyond the yield limit. Upon a decrease of the applied forcing a clear hysteresis in the dependence of each of the measured quantities on the applied pressure drop is observed. This finding comes into a perfect agreement with the yielding scenario recently proposed by Putz et al. (Rheologica Acta 48(6), 2009).

CPP 37.9 Thu 18:45 Poster A

Mechanical Properties and Structure in Precipitated Colloidal Silica — •Miao Wang[1,2], Marcel Roth[1], H. Henning Winter[2], and Günter K. Auernhammer[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]University of Massachusetts, Amherst, MA, USA

The mechanical properties of colloidal systems strongly depend on structure and interaction potential. Inorganic precipitated silica-gels of various compositions, as widely used as filler in paints, cosmetics and polymers, show this phenomenon. To analyze the correlation between 3D-structure and mechanics we use combined measurements by confocal reflection microscopy, piezo-rheometry, and Couette rheometry. Samples get prepared in a low-viscosity sol state and then transfered into the measurement cell before gelation sets in. In-situ confocal reflection microscopy visualizes the formation of gel. Simultaneously, this process is studied with a piezo-rheometer, which allows dynamic mechanical measurements on samples of less than 100 micrometer thickness. The applied shear strain lies typically below 0.001 (absolute displacement smaller than 100 nm). Classical rheometer measurements with a Couette cell extend the data to lower frequencies. Depending on composition, we find a relaxation process (frequency dependent shear modulus) at low frequencies. This frequency dependence suggests the structural relaxation of the network structure at long times. Structure and properties depend on water content in the sample. An increased water fraction in the gel results in a finer and more connected network with longer relaxation time but lower plateau modulus.

CPP 37.10 Thu 18:45 Poster A

Structure Formation in Processed Cheese and Rheological Evaluation of Some Influencing Factors — •Yamen Edelby and

Bernhard Senge — Institut for Food Technology, Department of Food Rheology, TU Berlin

The objective of the present paper is to elucidate the effect of melting salt content, rotational speed, fat and water content on the structuring process of processed cheese. The structure formation was detected by using oscillation measurements by Rheometer MCR301. For temperature sweeps: Deformation = 10^{-3}, f = 1 Hz, cool-running 85-10 °C with a cooling rate of 1 K /min. The processed cheese was manufactured at laboratory scale by a knife mill, a water bath and an agitator with a paddle stirrer. By means of a basic concept (66,0 g Gouda, 28,0 g curd cheese, 6,0 g butter, 2,8 g JOHA S 9 (as melting salt), 13,6 g water), a processing sequence for the manufacturing of processed cheese was performed. The melting salt content of processed cheese was changed at 300 rpm. The rotational speed of the agitator was increased. Then, the fat and water content were examined and evaluated. Throughout the processing and for all the measurements, the storage modulus (G') was > the loss modulus (G"), which indicates the solid state properties with dominant elastic properties. The loss factor curves (tan δ curves) show a relative minimum at about 70 °C as peak 1, an absolute maximum at about 45 °C as peak 2 and a relative maximum at 10-15 °C as peak 3. The best result of the optimization steps that will be made are: Melting salt content: 3.0 g, Rotational speed: 900 rpm, Fat content: 50%, Water content: 50%

CPP 38: Focus: Rheology II (joint focus with DRG)

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

Invited Talk CPP 38.1 Fri 9:30 C 130

The Rheology of Biological Cells — Mathias Sander[1], Benjamin Tränkle[1], Pablo Fernandez[2], Pramod Pullarkat[2], Lutz Heymann[3], Nuri Aksel[3], and •Albrecht Ott[1,2] — [1]Biologische Experimentalphysik, Universität des Saarlandes, Saarbrücken, Germany — [2]former address: Experimentalphysik 1, Universität Bayreuth, Bayreuth, Germany — [3]Technische Mechanik und Strömungsmechanik, Universität Bayreuth, Bayreuth, Germany

The mechanical properties of biological cells are important for many biological processes, among them embryogenesis, wound-healing and cancer. They are determined by the cytoskeleton, an active polymer gel, whose properties are poorly understood. Here we study cell rheological properties using a home built, single-cell rheometer. It consists of a single cell that is suspended between two parallel plates of cell-size. We observe that active and passive cell mechanical properties are clearly separated by their timescales. We show that the passive properties can be decomposed into a linear superposition of an elastic and a plastic response. While the elastic response can be easily understood from the mechanical properties of the cell cytoskeleton, the plastic response remains difficult to understand given current molecular knowledge. We present a novel technique, cell monolayer shearing. Here we create a single layer of about 10^6 isolated cells that adhere to the top and bottom plates of a standard rheometer. We use Fourier transform rheology to determine the degree of nonlinearity of the cell mechanical response. We show that we can assess cell adhesion-rupture in a very quantitative way. We present other interesting applications.

CPP 38.2 Fri 10:00 C 130

Rheological and (di)electric measurements on biopolymers, like blood systems — •Angelika Bender, Ulrich Förter-Barth, and Prof. Peter Eyerer — Fraunhofer Institute for Chemical Technology ICT, Pfinztal, Germany

In medical devices, like stents, being implanted into human body or dialysis apparatus transporting human blood, it is important to prevent clot formation. We have developed a method for detecting and monitoring blood coagulation and clot formation, said method enabling immediate intervention for clot destroying.

For the purpose of verification of (di)electric effects known for Naphtalin, water and polymers, oscillatory rheological measurements on coagulating blood have been combined with parallel electric measurement by means of an electrometer triggered by rheometer software as well as with parallel dielectric measurements.

Coagulation of blood being a viscoelastic liquid can be monitored by rheological measurements. Coagulation of blood as a biopolymer comprises formation of a haemostatic clot of fibrin. The measured electric signal coincide with curves characterising the coagulation of the blood probe, storage modulus for rheological measurements, and indicates start, progress and end of coagulation of the blood probe.

CPP 38.3 Fri 10:15 C 130

Competition of inertia and deformability - lateral motion of deformable particles in duct flow — •Timm Krüger, Badr Kaoui, and Jens Harting — Eindhoven University of Technology, Eindhoven, The Netherlands

The lateral motion of deformable particles in a planar Poiseuille flow has not been entirely understood. On the one hand, it is known that the deformability of particles (expressed by the capillary number, Ca, the ratio of viscous fluid and elastic particle stresses) promotes a migration towards the centerplane of the flow in the absence of inertia (zero Reynolds number, Re = 0). On the other hand, inertia effects are responsible for an outward migration of rigid particles (Ca = 0) close to the centerplane. We present 3D simulation results for systems with both finite Ca and Re and discuss the interplay of inertia and deformability effects.

CPP 38.4 Fri 10:30 C 130

Chromatographic, spectroscopic and rheological characterization of long chain branching induced by thermo-oxidative degradation of low-density polyethylene — •Victor Hugo Rolon-Garrido[1], Martin Zatloukal[2,3], and Manfred H Wagner[1] — [1]Chair of Polymer Engineering/Polymer Physics, TU Berlin, Fasanenstrasse 90, D-10623 Berlin, Germany — [2]Polymer Centre, Faculty of Technology, Tomas Bata University in Zlin, TGM 275, Zlin 76272, Czech Republic — [3]Centre of Polymer Systems, University Institute, Tomas Bata University in Zlin, Nad Ovcirnou 3685, 760 01 Zlin, Czech Republic

Low-density polyethylene was thermo-oxidatively degraded, i.e. degraded in the presence of air, by a one thermal cycle (1C) treatment during times between 30 and 90 minutes, and by a two thermal cycles (2C) treatment, i.e. after storage at room temperature an already previously degraded sample was further degraded during times between 15 and 45 minutes. Changes in the molecular weight distribution were detected by GPC and the intrinsic viscosity. Branching was confirmed by FTIR measurements. The enhanced strain hardening effect observed in uniaxial extension experiments presents a decisive evidence for an increased long-chain branching (LCB) content in both 1C and 2C samples. Elongational viscosity data were analyzed by the MSF and the Wagner-I model. It can be stated that elongational rheology is a powerful method to detect structural changes due to thermo-oxidative degradation.

CPP 38.5 Fri 10:45 C 130

Carbon dioxide plasticized polymer melts - An interpretation by means of the free volume concept — •Bernadette Duscher[1,2], Alois Schausberger[2], and Wolfgang Stadlbauer[1] — [1]Transfercenter für Kunststofftechnik GmbH, Franz-Fritsch Str. 11, A-4600 Wels — [2]Johannes Kepler University, Altenberger Str. 69, A-4040 Linz

CO_2 is a well established physical foaming agent for polymers. However, dissolving carbon dioxide under pressure strongly affects the rheological properties of the melt. The influence of pressure and of low molecular weight diluents ($M<M_c$) on the material functions are determined via oscillatory measurements. Therefore, a common plate-plate-system in a pressure cell is used. Relations based on the free volume concept are used to interpret the experimental results. In case of linear polymers (PS, PP) the time-concentration-superposition is simple. The mastercurve is created by shifting the dynamic moduli of the CO_2-diluted polymer melt to the dynamic moduli of the neat polymer. The shift factors obtained are corrected by the effect of pressure. In addition, by use of the generalized Doolittle relation the concentration dependent horizontal shift factors a_c are calculated. The rheological properties of carbon dioxide plasticized polymer melts as well as the molar plasticizing activity A of an additive can be predicted.

Independently of the horizontal shift a_c, an additional shift b_c on the modulus axis is found by a vanGurp-Palmen plot. The relation

$b_c = w^2$ is applied and the vertical shifts are calculated. w is the weight fraction of the entangled polymer.

CPP 38.6 Fri 11:00 C 130

A sequence of physical processes determined and quantified in LAOS: A quantitative approach — •Simon Rogers — Forschungszentrum Jülich, Jülich, Germany

An entirely new way of analyzing linear and nonlinear oscillatory material responses is presented. The new quantitative sequence of physical processes (SPP) method is based on viewing generic nonlinear responses as sequences of 2D planes imbedded in a 3D space defined by the strain, strain-rate, and stress axes. Associated with each plane is a normal vector that wholly determines its orientation, which can be used to gain physically meaningful information by calculating the angles between a modified form of the normal vector and two reference vectors. Using this analysis technique, time-dependent phase and complex modulus, or dynamic modulus, information is obtainable throughout a period for arbitrary oscillatory responses. The new technique is applied to the Bingham plastic model, model power-law fluids, the Hershel-Bulkley model, and the nonlinear Giesekus model, to accustom the audience to its function.

CPP 38.7 Fri 11:15 C 130

Microscopic relaxation processes in branched/linear polymer blends by Rheo-Sans — •Nino Ruocco[1], Wim Pyckhout Hintzen[1], Aurel Radulescu[1], Dieter Richter[1], Peter Lindner[2], and Daniel Read[3] — [1]Forschungszentrum Jülich, JCNS-1, Jülich, Germany — [2]Institut Laue-Langevin, Grenoble, France — [3]Department of Applied Mathematics, University of Leeds, UK

The present study focuses on the hierarchical relaxation processes in a cayley-tree polymer, dispersed in linear polyisoprene (PI) using a Rheo-SANS combination. The introduction of branching points, which join different generations, and the dynamics of the embedding linear matrix have a huge impact in the dynamic relaxation spectrum. Molecular variables that are relaxed on the time scale of experiment and those, which are frozen or quenched, can be distinguished. Within a RPA treatment, taking into account the different degrees of freedom, the observed loss of anisotropy after a fast step strain can be correlated with the fast relaxation of the outer arms and a slow one for the inner section: a hierarchical relaxation from the tips inwards to the branching point leads to isotropization of the chain ends with loss of orientation in a diluted tube. Microscopic access to relaxation processes and the corresponding structural parameters is enabled through uniaxial step strain experiments at strain rates faster than their inverse relaxation time. The parameter space is scanned by appropriate SANS experiments in the respective time domains, which uniquely resolve the difficulties in extracting dynamics of the minority component from macroscopic rheology, which is dominated by the matrix.

CPP 38.8 Fri 11:30 C 130

Investigation of the Miscibility and Phase Separation of Molten PP/PE Blends via Rheometry — •Matthias Mihalic and Alois Schausberger — Institute of Polymer Science, Johannes-Kepler-Universität, A-4040 Linz, Austria

Rheometry is a powerful tool for the detection of phase separation in molten polymers and thus for the investigation of the solubility of each component in a mixture. The sample preparation for such measurements typically involves one or several crystallization steps, which in turn induce phase separation in the sample. Neither will this phase separation be balanced out by diffusion in the melt, nor is the rheometer suitable to be used as a compounder. Consequently, one might get somewhat distorted results. Therefore it seems desirable to avoid any crystallization between the compounding and the rheological characterization of a blend.

To this end, an experimental set-up was designed such that after compounding, the molten blends are directly injected into the measuring cell of a rheometer, where the dynamic moduli are determined.

In case of miscibility, the relaxation time spectrum of a blend can be simply calculated from the combined molar mass distributions of the components. Otherwise, phase separation will be reflected in the spectrum of the mixture obtained from dynamic mechanical data. The measurement results are further analyzed using the model of Gramespacher and Meissner in order to gain information about the phase structure of the blend. In addition, by preparing blends of different concentrations, the boundaries of miscibility are checked.

CPP 38.9 Fri 11:45 C 130

Influence of carbon dioxide on the viscoelastic properties of polystyrene melts — •Ulrich A. Handge[1,2] and Volker Altstädt[1] — [1]Department of Polymer Engineering, Faculty of Engineering Science, University of Bayreuth, Universitätsstraße 30, 95447 Bayreuth — [2]Helmholtz-Zentrum Geesthacht, Institute of Polymer Research, Max-Planck-Strasse 1, 21502 Geesthacht

The addition of carbon dioxide to polystyrene strongly influences the viscoelastic properties of polystyrene. Carbon dioxide is dissolved in the polymer matrix and acts as a plasticizer. Generally, the glass transition temperature and the viscosity of polystyrene/carbon dioxide solutions decrease with increasing carbon dioxide concentration. In this work, the linear viscoelastic properties of solutions of polystyrene melts with carbon dioxide are investigated. A rotational rheometer which is equipped with a pressure cell allows one to perform experiments using a plate-plate rheometry. The pressure cell can be filled with the blowing agent carbon dioxide, and torque and normal force are transferred via a magnetic coupling to the measurement head of the rheometer. We study the transient shear rheology and test superposition principles of the rheological properties with respect to time, temperature, pressure and concentration of the blowing agent. These measurements allow us to analyze the linear viscoelastic properties of polystyrene/carbon dioxide solutions, in particular the influence of carbon dioxide on the average relaxation time of polystyrene. Our data indicate that glass transition temperature and average relaxation time of polystyrene are strongly influenced by the addition of carbon dioxide.

CPP 38.10 Fri 12:00 C 130

An in-situ investigation of the draw resonance phenomenon in film casting of a polypropylene melt — Teodor Burghelea[1], Hans Jurgen Griess[2], and •Helmut Muenstedt[2] — [1]Universite de Nantes, Nantes Atlantique Universites, CNRS, Laboratoire de Thermocinetique de Nantes, UMR 6607, La Chantrerie, Rue Christian Pauc, B.P. 50609, F-44306 Nantes Cedex 3, France — [2]Institute of Polymer Materials, Friedrich-Alexander-University Erlangen-Nu *rnberg, D-91058 Erlangen, Germany

An experimental investigation of the stability of the casting process of a polypropylene film is presented. Several flow regimes are identified: stable, oscillatory and chaotic. Measurements of the velocity distribution along and across the extruded film corresponding to each drawing regime are presented. The intermittent physical rupture of the film's edges observed within the chaotic drawing regime is explained by the emergence of a "V - shaped" region of high axial gradients of the axial velocity component which indicates a highly inhomogeneous distribution of tensile stresses. By measurements of the statistics of the fluctuations of both the film's width and velocity a continuous (second order) imperfect bifurcation towards oscillatory states is found. The fluctuation data acquired before the chaotic regime is reached can be fitted by the stationary Landau-Ginsburg equation. The observation of a stable limit cycle at the onset of the bifurcation identifies it as a supercritical Hopf bifurcation. The experimentally found scaling of the onset and amplitude of the bifurcation with the Weissenberg number indicates that elasticity destabilizes the drawing process.

CPP 39: Wetting, Micro and nanofluidics II

Time: Friday 9:30–12:00 Location: C 243

CPP 39.1 Fri 9:30 C 243

Capillary Levelling in Thin Polymer Films as a Nano-Rheological Tool to Probe Interface Dynamics — •Oliver Bäumchen, Joshua D. McGraw, Melissa Ferrari, Paul D. Fowler, and Kari Dalnoki-Veress — Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, L8S 4M1

Entanglement of polymer chains in confinement is modified as a result of altered chain conformations. According to Silberberg's principle, chain segments are reflected at an interface causing a reduction of the inter-chain entanglement density. If the interface is transient, local polymer conformation changes can be inferred from a temporal change in flow properties: over time polymer chains become more entangled, thus there is more resistance to flow. Here, we measure the gradual disappearance of an entropic interface between two melts of identical polymer chains during the flow of stepped bilayer polymer films. Samples are prepared in the glassy state and, when in the melt, flow to relieve the Laplace pressure gradient induced by a step in the topography (McGraw et al., Soft Matter, 2011). Our results reveal the dynamics of re-entanglement across the transient entropic interface.

CPP 39.2 Fri 9:45 C 243

Impact of polystyrene chain length on the instability of a dewetting liquid front — •Sabrina Haefner[1], Matthias Lessel[1], Ludovic Marquant[1], Oliver Bäumchen[2], and Karin Jacobs[1] — [1]Saarland University, Experimental Physics, D-66041 Saarbrücken, Germany — [2]McMasters University, Dept. of Physics & Astronomy, Hamilton, ON, Canada

A water cylinder in air is breaking up in droplets, seeking to minimize its surface energy. This phenomenon is known as Rayleigh-Plateau-instability. A liquid front of a dewetting liquid film is a similar geometry and hence also subject to the Rayleigh-Plateau-instability. For polymer melts Marquant et al. have shown the influence on the instability by the type of solid/liquid boundary condition ('slip' or 'no slip'). Bäumchen et al. have shown in a recent study, that in thin polystyrene (PS) films slippage can be induced by only exceeding a certain chain length of the polymer. Combining both things, we are interested in the impact of chain-length-induced slippage on the Rayleigh-Plateau-instability of a dewetting front. As substrates an amorphous fluoropolymer (AF1600) layer was prepared on smooth Si wafers entailing nearly no-slip conditions for PS chain length under 35 kg/mol. With increasing slip length the instability sets in at lower dewetted distances. At a certain molecular weight (higher slippage) this is reversed and the instability then develops only after larger dewetted distances. This effect can be explained by the rim profile of the liquid front, which is strongly influenced by the type of boundary condition.

CPP 39.3 Fri 10:00 C 243

Orientational prewetting of planar solid substrates by a model liquid crystal — •Manuel Greschek and Martin Schoen — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Fakultät für Mathematik und Naturwissenschaften, Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany

We present grand canonical ensemble Monte Carlo simulations of prewetting transitions in a model liquid crystal at structureless solid substrates. Molecules of the liquid crystal interact via anisometric Lennard-Jones potentials and can be anchored planar or homeotropically at the substrates. Fluid-substrate attraction is modeled by a Yukawa potential of variable range. By monitoring the grand-potential density and the nematic order parameter as functions of the chemical potential several discontinuous prewetting, wetting, and isotropic-nematic phase transitions are observed. These transitions depend on both the range of the fluid-substrate attraction and the specific anchoring at the substrate. Our results show that at substrates characterized by degenerate anchoring prewetting occurs at lower chemical potentials compared with cases in which the anchoring is monostable. This indicates that prewetting transitions are driven by orientational entropy because degenerate anchoring allows for more orientationally distinct configurations of molecules compared with monostable anchoring. By analyzing in addition local density and various local order parameters a detailed picture of the structure of various phases emerges from our simulations.

Topical Talk CPP 39.4 Fri 10:15 C 243

Guided and spatio-selective transport via anisotropic fluid flows — •Anupam Sengupta and Christian Bahr — Max-Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany

Microscale flow of anisotropic fluids [1,2] (nematic liquid crystals) offers a novel approach in the realm of transport phenomena. We study the transport of colloidal particles, either isolated or self-assembled chains, flowing in a nematic matrix through microfluidic channels. We demonstrate the influence of the nematic director field on the spatial orientation of the particles and the guidance of the particles by flow-induced topological defect structures of the nematic matrix. The transport of colloidal entities can be additionally tuned using an external field or by means of smart microfluidic architecture. In addition to flow parameters and channel dimensions and geometry, significant influence of the equilibrium molecular orientation of the liquid crystal on the channel walls (surface anchoring) has been observed. Surface anchoring of the molecules affects the evolution and sustenance of flow-induced phenomena in liquid crystals. This plays a pivotal role in the transport process, effectively providing us the route to guided and/or stereo-selective transport of colloidal particles over large length scales. Such phenomena are in contrast to isotropic fluids. The transport phenomena are characterized using a combination of polarising optical microscopy and fluorescence confocal polarizing microscopy.

[1] A. Sengupta, S. Herminghaus and Ch. Bahr, Mol. Cryst. Liq. Cryst. **547**, 203 (2011).
[2] A. Sengupta, U. Tkalec and Ch. Bahr, Soft Matter **7**, 6542 (2011).

CPP 39.5 Fri 10:45 C 243

Inertial Lift Forces and Probability Distributions in InertialMicrofluidics — •Christopher Prohm, Michael Gierlak, and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin, Germany

At intermediate Reynolds numbers, particles in a microfluidic channel organize themselves at a fixed distance from the channel axis and its walls[1]. This effect can be described in terms of an effective lift force acting on the particles. Devices utilizing this inertial focusing for particle separation have recently been demonstrated[2,3].

Here, we study a spherical particle in a pressure driven flow through a microchannel at intermediate Reynolds numbers. We employ multi-particle collision dynamics[4] (MPCD) to simulate the particle motion coupled to a viscous fluid which is described by the full Navier-Stokes equation. MPCD is a mesoscale simulation technique and has successfully been applied to colloidal dynamics in previous studies.

We determine lift forces and resulting single particle probability distributions in steady state and analyze their dependence on particle radius and Reynolds number. To connect lift forces and distributions, we propose a Smoluchowski equation, where the point particle exhibits a drift motion due to the lift force. We show that this effective picture and the simulations are in good agreement.

[1] Segré and Silberberg, *Nature*, **189**, 209 – 210 (1961).
[2] Hur et al., *Lab Chip*, **10**, 274 – 280 (2009).
[3] Di Carlo et al., *PNAS*, **104**, 18892 – 18897 (2007).
[4] Kapral et al., *Adv. Chem. Phys.*, **140**, 89 – 146 (2008).

CPP 39.6 Fri 11:00 C 243

Sorting of chiral particles in microfluidic devices with helical flows — •Maria Zvyagolskaya[1], Ralf Eichhorn[2], and Clemens Bechinger[1] — [1]Universität Stuttgart, 2. Physikalisches Institut, Pfaffenwaldring 57, 70569 Stuttgart — [2]NORDITA, Roslagstullsbacken 23, 106 91 Stockholm, Sweden

Different enantiomers of chiral compounds often show huge differences in their biochemical activity. Therefore, the separation of such molecules which are typically produced in equal amounts during synthesis, is important for many processes e.g. in pharmaceutical or food industry. Current separation techniques are frequently based on differences in the migration behaviour in chiral host media. However, such materials are expensive and have to be optimized for different chiral compounds. Here, we demonstrate with experiments and simulations a novel method which is based on hydrodynamic coupling of chiral compounds in a helical fluid flow. Three-dimensional chiral particles on the micron-scale are created by a photolithography and are labeled with different fluorescent dyes to distinguish their chirality. In the presence of a helical flow, we observe marked differences in the behavior of particles with opposite chirality regarding their spatial distribution perpendicular to the flow which leads to an effective separation mechanism.

CPP 39.7 Fri 11:15 C 243

Rotating magnetic field assisted microfluidics — •Frank Wittbracht[1], Bernhard Eickenberg[1], Alexander Weddemann[2], and Andreas Hütten[1] — [1]Thin Films and Physics of Nanostructures, Bielefeld University, Bielefeld, Germany — [2]Research Laboratory of Electronics/LEES, MIT, Cambridge, United States

Superparamagnetic beads suspended in a liquid show characteristic behavior when immersed in a homogenous external magnetic field. Due to the inhomogeneous character of the stray field of the beads, magnetic agglomerates are formed. The dimensionality of these magnetic superstructures can be adjusted by rotating the external magnetic field. This allows especially for the formation of highly ordered two-dimensional clusters consisting of magnetic beads [1]. Time scales for the cluster formation are studied with respect to a dependence on the rotation frequency of the magnetic field [2]. We present a microfluidic device, which utilizes the interaction between magnetic agglomerates and channel walls in order to perform colloidal separation. The magnetic agglomerates may also act as dynamic free-flowing microstirrers which enhance the effective diffusion at the interface of a two fluid streams. At the chosen system parameters an increase in the diffusivity of 32 was obtained and a separation efficiency of about 80% at flow rates up to 0.4 mm/s was achieved.

[1] A. Weddemann, F. Wittbracht, B. Eickenberg, A. Hütten, Langmuir, 26, 19225 (2010)

[2] F. Wittbracht, B. Eickenberg, A. Weddemann, A. Hütten, J. Appl. Phys., 109, 114503 (2011)

CPP 39.8 Fri 11:30 C 243

Hydration of small hydrophobic objects: The effects of an electric field — •Zoran Miličević[1], David M. Smith[2], and Ana-Sunčana Smith[1] — [1]Institut für Theoretische Physik and Cluster of Excellence: Engineering of Advanced Materials, Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Computer Chemie Centrum, Universität Erlangen-Nürnberg, Erlangen, Germany

It is well established that the hydrophobicity of an interface, droplet or a particle can be modulated by an external electric field. However, the field effects on water structure around a hydrophobic object are not understood to a satisfactorily level. We study the organization of water around a Lennard-Jones particle and an oil droplet in the presence and absence of a static electric field. We perform extensive MD simulations using the GROMACS software package and the SPC/E model of water. The structure of water is analyzed by means of the total solute-solvent correlation function, which includes the orientational degrees of freedom of the solvent. We find that a structure of water arises from the competition between optimal orientation of water with respect to the field and with respect to the solute, yielding an asymmetric distribution of solvent charges around the particle. The particle thus appears to be a small dipole. Another consequence of the field are very long range solvent-solute effective interactions. We furthermore evaluate the force correlations as a function of time and find them sensitive to the treatment of van der Waals interactions in simulations, which may explain some discrepancies in the observed mobilities of small droplets in simulations reported previously in the literature.

CPP 39.9 Fri 11:45 C 243

Theory of water and charged liquid bridges — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP) Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

The phenomena of liquid bridge formation due to an applied electric field is investigated. A new solution of a charged catenary is presented which allows to determine the static and dynamical stability conditions where charged liquid bridges are possible. The creeping height, the bridge radius and length as well as the shape of the bridge is calculated showing an asymmetric profile in agreement with observations. The flow profile is calculated from the Navier Stokes equation leading to a mean velocity which combines charge transport with neutral mass flow and which describes recent experiments on water bridges. arXiv:1107.0459