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

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Overview of Invited Talks, Topical Talks and Sessions

(lecture rooms ZEU 222, ZEU 160, and ZEU 114; Poster P1 and P2)

Invited and Topical Talks of CPP Sessions (excluding Focused Sessions)

CPP 2.1	Mon	10:30–11:00	ZEU 222	**Crayfish combine amorphous and crystalline mineral to build a functional tooth structure** — •Barbara Aichmayer, Shmuel Bentov, Ali Al-Sawalmih, Admir Masic, Paul Zaslansky, Peter Fratzl, Amir Sagi, Amir Berman
CPP 5.1	Mon	14:00–14:30	ZEU 222	**Light harvesting in single polymer chains and inorganic nanostructures** — •John M. Lupton
CPP 6.7	Mon	15:45–16:15	ZEU 160	**Charge-Controlled Protein Crystallization** — •Fajun Zhang, Georg Zocher, Andrea Sauter, Marcell Wolf, Felix Roosen-Runge, Thilo Stehle, Frank Schreiber
CPP 12.1	Tue	10:30–11:00	ZEU 222	**Modelling charge transport in organic semiconductors** — •Denis Andrienko
CPP 14.1	Tue	10:30–11:00	ZEU 114	**Network effects in nano-filled polymer systems** — •Kay Saalwächter, Cornelius Franz, Kerstin Schäler, Salim Ok, Martin Steinhart, Aurelie Papon, Francois Lequeux, Helene Montes
CPP 17.1	Tue	14:00–14:30	ZEU 114	**Modulated mesophases: from labyrinths to liquid ferroelectric chords.** — •Alexey Eremin, Ulrike Kornek, Ralf Stannarius, Antal Jákli, Hideo Takezoe
CPP 25.1	Wed	10:30–11:00	ZEU 222	**From elementary building blocks towards colloidal molecules** — Claudia Simone Wagner, •Alexander Wittemann
CPP 31.1	Wed	14:00–14:30	ZEU 222	**Control of Charge Carrier Dynamics in Disordered Conjugated Polymers** — •Dirk Hertel
CPP 39.9	Thu	12:30–13:00	ZEU 222	**Combining structure and mechanical properties of colloidal systems** — Marcel Roth, Chris Grigoriadis, Jinyu Zhao, Burkhard Mayer, Doris Vollmer, George Floudas, •Günter. K. Auernhammer
CPP 40.1	Thu	10:30–11:00	ZEU 160	**Crystallization in block copolymer thin films** — •Christine M. Papadakis, Charles Darko, Günter Reiter
CPP 41.1	Thu	10:45–11:15	ZEU 114	**Local Anisotropy of Fluids, Glasses and Jammed Bead Packs** — •Gerd Schroeder-Turk
CPP 41.7	Thu	12:30–13:00	ZEU 114	**Concentration fluctuations and intrinsic confinement effects in binary glass forming liquids: Insights from neutron scattering and X-ray photon correlation spectroscopy** — •Thomas Blochowicz, Sebastian Schramm, Emmanuel Gouirand, Philipp Gutfreund, Bernd Stühn, Bernhard Frick, Yuriy Chushkin
CPP 43.1	Thu	14:00–14:30	ZEU 222	**NanoModel - Multi-Scale Modelling of Nano-Structured Polymeric Materials** — •Horst Weiss
CPP 43.15	Thu	18:00–18:30	ZEU 222	**Are nanomaterials safe? Physico-chemical characterization for regulation and for life-cycle assessment of nanocomposites** — •Wendel Wohlleben
CPP 46.1	Fri	10:30–11:00	ZEU 222	**Droplet-based microfluidics and the dynamics of emulsions** — •Jean-Christophe Baret

Invited Talks of the Tutorial “Physics with neutrons – from proteins via polymer thin films to spin waves”

See Tutorials for the full program. (organizer: C. Papadakis)

CPP 1.1	Sun	16:00–16:45	HSZ 403	**Neutrons as a sensitive tool to investigate nano- and mesostructured materials** — •Stephan Förster
CPP 1.2	Sun	16:45–17:30	HSZ 403	**Reflectivity and GISAS** — •Roland Steitz
CPP 1.3	Sun	17:45–18:30	HSZ 403	**Neutron spectroscopy on solids** — •Astrid Schneidewind

Invited Talks of the SKM-Symposium “Elementary Processes in Organic Photovoltaics” (SKM-SYOP)

See SKM-SYOP for the full program of the Symposium.

SKM-SYOP 1.1	Mon	10:30–11:00	TRE Ma	**Charge separation in organic solar cells and the principle of detailed balance** — •Uwe Rau, Thomas Kirchartz
SKM-SYOP 1.2	Mon	11:00–11:30	TRE Ma	**Three-Dimensional Nanoscale Organization of Bulk Heterojunction Polymer Solar Cells** — •Joachim Loos
SKM-SYOP 1.3	Mon	11:30–12:00	TRE Ma	**Reliable prediction of charge transfer excitations using optimally tuned range-separated hybrid functionals** — •Leeor Kronik
SKM-SYOP 1.4	Mon	12:00–12:30	TRE Ma	**Charge separation and recombination in organic solar cells** — •James Durrant
SKM-SYOP 1.5	Mon	12:30–13:00	TRE Ma	**Efficient and stable organic vacuum deposited p-i-n-type tandem solar cells** — •Martin Pfeiffer

Invited Talks of the Focused Sessions “Confinement of Polymers in Nanoscopic Layers - How Much do Properties Change?”

Properties of polymers forced into the one-dimensional confinement of nanometric thin layers are a cutting-edge and -in part- highly controversial topic of current polymer research. Some of the open questions are of quite fundamental nature. It is the aim of this Focus-Session to bring together the exponents of the different views and to compare and discuss the experimental and theoretical findings on the influence of confinement and interfacial interactions on structural and dynamic properties and the glass transition of polymers confined in thin layers.(organizers: G. Reiter and M. Stamm)

CPP 13.1	Tue	10:30–11:00	ZEU 160	**Rheological Response of Ultrathin Polymer Films** — •Gregory McKenna, Paul O’Connell, Jinhua Wang
CPP 13.2	Tue	11:00–11:30	ZEU 160	**Molecular dynamics at nanometric length-scales** — •Friedrich Kremer
CPP 13.3	Tue	11:30–12:00	ZEU 160	**On the origin of the deviations from bulk behavior in ultrathin polymer films: from glass transition to tracer diffusivity** — •Simone Napolitano, Michael Wübbenhorst, Cinzia Rotella
CPP 13.4	Tue	12:00–12:30	ZEU 160	**Calorimetry of Thin Films – From Single Layer Glass Transitions to Inter-layer Diffusion in Double Layers** — •Christoph Schick, Dongshan Zhou, Heiko Huth
CPP 16.1	Tue	14:00–14:30	ZEU 160	**Glass Transition Dynamics of Polymer Films** — •Ophelia K. C. Tsui
CPP 16.2	Tue	14:30–15:00	ZEU 160	**Conformational properties of polymer melts in spatial confinement** — Hendrik Meyer, Albert Johner, Joachim Wittmer, Julia Zabel, Jean Farago, •Jörg Baschnagel

Invited Talks of the Intersectional Symposium "Transport and Spectroscopy in Molecular Nanostructures" (SYMN)

See SYMN for the full program of the Symposium.

SYMN 1.1	Wed	10:30–11:00	HSZ 01	**Exciton localization and dynamics in molecular aggregates** — •Jasper Knoester
SYMN 1.2	Wed	11:00–11:30	HSZ 01	**Spectroscopy and transport in carbon nanotubes and graphene nanoribbons for electronics and biological applications** — •Oleg Prezhdo
SYMN 1.3	Wed	11:30–12:00	HSZ 01	**Multidimensional Optical Spectroscopy of Biological Complexes** — •Shaul Mukamel
SYMN 1.4	Wed	12:00–12:30	HSZ 01	**Theory of light-harvesting in photosynthetic pigment-protein complexes** — •Thomas Renger, Marcel Schmidt am Busch, M. El-Amine Madjet, Frank Müh
SYMN 1.5	Wed	12:30–13:00	HSZ 01	**How do algae use quantum mechanics to harvest light for photosynthesis?** — •Gregory Scholes

Invited Talks of the Focused Session "Computational Polymer Physics – New Developments"

The increasing power of modern computers and the development of new models and techniques enhances the importance of computer simulations for investigating complex polymer systems and to solve long-standing questions in polymer science. The aim of this focus-session is to present the state of the art of computational polymer physics to a broader audience. The session covers different approaches to polymer systems starting from techniques which model the specific details of polymers, self-consistent field methods, exact sampling methods and new MC and MD approaches to soft matter problems. (organizer: J.-U. Sommer)

CPP 33.1	Wed	14:00–14:30	MOL 213	**Multiscale Simulation of Soft Matter: Challenges** — •Florian Müller-Plathe
CPP 33.2	Wed	14:30–15:00	MOL 213	**A self-consistent field approach for crosslinked polymer materials** — •Friederike Schmid
CPP 33.3	Wed	15:00–15:30	MOL 213	**Mechanical separation of short double stranded DNA: Effect of pulling geometry** — •Sanjay Kumar
CPP 33.4	Wed	15:45–16:15	MOL 213	**Soft coarse-grained models for multi-component polymer melts** — •Marcus Müller
CPP 33.5	Wed	16:15–16:45	MOL 213	**Simulations of Polymer Electrolytes for Lithium-Ion Batteries Highly Accurate Polarizable Potentials** — •Grant Smith

Invited Talks of the SKM-Symposium Heterogenous Nucleation and Microstructure Formation: Steps towards a System and Scale-bridging Understanding" (SKM-SYMF)

See SKM-SYMF for the full program of the Symposium.

SKM-SYMF 1.1	Thu	14:30–15:00	TRE Ma	**Visualizing the structural solid-liquid transition with colloidal suspensions** — •Peter Schall
SKM-SYMF 1.2	Thu	15:00–15:30	TRE Ma	**Crystallization process in suspensions of hard spheres** — •Tanja Schilling, Hans-Joachim Schoepe, Martin Oettel, George Opletal, Ian Snook
SKM-SYMF 1.3	Thu	15:30–16:00	TRE Ma	**Homogeneous bulk, surface, and edge nucleation in crystalline nanodroplets** — •Kari Dalnoki-Veress, Jessica Carvalho
SKM-SYMF 1.4	Thu	16:00–16:30	TRE Ma	**Polymer Crystallization: Ordered Structures in Complex Systems** — •Jens-Uwe Sommer
SKM-SYMF 1.5	Thu	16:30–17:00	TRE Ma	**Phase formation and microstructure development in multicomponent alloys** — •Jürgen Eckert

Sessions

CPP 1.1–1.3	Sun	16:00–18:30	HSZ 403	**Tutorial: Physics with neutrons - from proteins via polymer thin films to spin waves**
CPP 2.1–2.9	Mon	10:30–13:00	ZEU 222	**Biopolymers and Biomaterials I (jointly with BP)**
CPP 3.1–3.10	Mon	10:30–13:00	ZEU 160	**Interfaces and Thin Films I**
CPP 4.1–4.5	Mon	10:15–13:00	HSZ 103	**Focus Session "Nanoparticles, Nanocrystals and Colloids" (jointly with MA)**
CPP 5.1–5.12	Mon	14:00–17:30	ZEU 222	**Organic Semiconductors I: Solar Cells A (jointly with HL, DS)**
CPP 6.1–6.12	Mon	14:00–17:30	ZEU 160	**Charged Soft Matter**
CPP 7.1–7.13	Mon	14:00–17:30	ZEU 114	**Interfaces and Thin Films II**
CPP 8.1–8.53	Mon	17:30–19:30	P2	**Poster: Organic Semiconductors**
CPP 9.1–9.10	Mon	17:30–19:30	P2	**Poster: Biopolymers and Biomaterials**
CPP 10.1–10.11	Mon	17:30–19:30	P2	**Poster: Charged Soft Matter**
CPP 11.1–11.19	Mon	17:30–19:30	P2	**Poster: New Instruments and Methods**
CPP 12.1–12.9	Tue	10:30–13:00	ZEU 222	**Organic Semiconductors II: Solar Cells B (jointly with HL, DS)**
CPP 13.1–13.6	Tue	10:30–13:00	ZEU 160	**Focused Session: Confinement of Polymers in Nanoscopic Layers - How Much do Properties Change? I**
CPP 14.1–14.9	Tue	10:30–13:00	ZEU 114	**Elastomers and Gels**
CPP 15.1–15.5	Tue	14:00–15:15	ZEU 222	**Organic Semiconductors III: Aggregation and Nanostructures (jointly with HL, DS)**
CPP 16.1–16.4	Tue	14:00–15:30	ZEU 160	**Focused Session: Confinement of Polymers in Nanoscopic Layers - How Much do Properties Change? II**
CPP 17.1–17.4	Tue	14:00–15:15	ZEU 114	**Liquid Crystals**
CPP 18.1–18.9	Tue	18:00–20:00	P1	**Poster: Transport and Spectroscopy in Molecular Nanostructures (Intersectional Session with MO)**
CPP 19.1–19.24	Tue	18:00–20:00	P2	**Poster: Interfaces and Thin Films**
CPP 20.1–20.5	Tue	18:00–20:00	P2	**Poster: Computational Soft Matter Physics**
CPP 21.1–21.8	Tue	18:00–20:00	P2	**Poster: Confinement of Polymers in Nanoscopic Layers - How Much do Properties Change?**
CPP 22.1–22.9	Tue	18:00–20:00	P2	**Poster: Glass Transition and Dynamics of Liquids**
CPP 23.1–23.17	Tue	18:00–20:00	P2	**Poster: Semicrystalline Polymers, Polymer Crystallization and Self-Assembly**
CPP 24.1–24.7	Tue	18:00–20:00	P2	**Poster: Polymer Dynamics**
CPP 25.1–25.9	Wed	10:30–13:00	ZEU 222	**Colloids and Complex Liquids I - Structure**
CPP 26.1–26.5	Wed	10:30–11:45	ZEU 160	**Polymer Dynamics**
CPP 27.1–27.4	Wed	12:00–13:00	ZEU 160	**Polymer Self Assembly**
CPP 28.1–28.9	Wed	10:15–13:00	ZEU 260	**Biopolymers and Biomaterials II (jointly with BP)**
CPP 29.1–29.10	Wed	15:00–17:45	ZEU 260	**Biopolymers and Biomaterials III (jointly with BP)**
CPP 30.1–30.11	Wed	10:15–13:00	KÖN Farb	**Glasses and Glass Transition I (jointly with DY, DF)**
CPP 31.1–31.10	Wed	14:00–17:00	ZEU 222	**Organic Semiconductors IV: Excitations and Charges (jointly with HL, DS)**
CPP 32.1–32.11	Wed	14:00–17:00	ZEU 160	**Transport and Spectroscopy in Molecular Nanostructures I (related to SYMN, jointly with MO)**
CPP 33.1–33.5	Wed	14:00–16:45	MOL 213	**Focused Session: Computational Polymer Physics - New Developments (jointly with DY)**
CPP 34.1–34.13	Wed	17:00–19:00	P2	**Poster: Elastomers and Gels**
CPP 35.1–35.24	Wed	17:00–19:00	P2	**Poster: Micro- and Nanofluidics**
CPP 36.1–36.24	Wed	17:00–19:00	P2	**Poster: Nanoparticles and Composite Materials**
CPP 37.1–37.3	Wed	17:00–19:00	P2	**Poster: Heterogeneous Nucleation and Microstructure Formation (related to SYMF)**
CPP 38.1–38.37	Wed	17:00–19:00	P2	**Poster: Colloids and Complex Liquids**
CPP 39.1–39.9	Thu	10:30–13:00	ZEU 222	**Colloids and Complex Liquids II - Dynamics and Mechanical Properties**
CPP 40.1–40.9	Thu	10:30–13:00	ZEU 160	**Polymer Crystallization and Semicrystalline Polymers**
CPP 41.1–41.7	Thu	10:45–13:00	ZEU 114	**Glasses and Glass Transition II (jointly with DY, DF)**
CPP 42.1–42.10	Thu	10:30–13:00	TOE 317	**Transport and Spectroscopy in Molecular Nanostructures II (related to SYMN, jointly with CPP)**
CPP 43.1–43.15	Thu	14:00–18:30	ZEU 222	**Nanoparticles and Composite Materials I**
CPP 44.1–44.15	Thu	14:00–18:00	ZEU 160	**Micro- and Nanofluidics I**

CPP 45.1–45.3	Thu	17:15–18:00	ZEU 114	**Colloids and Complex Liquids III - External Fields**
CPP 46.1–46.9	Fri	10:30–13:00	ZEU 222	**Micro- and Nanofluidics II**
CPP 47.1–47.9	Fri	10:30–12:45	ZEU 160	**Heterogeneous Nucleation and Microstructure Formation (related to SYMF, jointly with MM)**
CPP 48.1–48.10	Fri	10:30–13:00	ZEU 114	**Nanoparticles and Composite Materials II**

Annual General Meeting of the Chemical and Polymer Physics Division

Mittwoch 19:15–20:00 ZEU 160

- Bericht
- Frühjahrstagung 2012
- Verschiedenes

CPP 1: Tutorial: Physics with neutrons - from proteins via polymer thin films to spin waves

Time: Sunday 16:00–18:30 Location: HSZ 403

Tutorial CPP 1.1 Sun 16:00 HSZ 403
Neutrons as a sensitive tool to investigate nano- and mesostructured materials — •Stephan Förster — University of Bayreuth, Fakultät für Chemie

Neutrons can be similarly used as x-rays to investigate the structure of nano- and mesoscale synthetic and biological materials. Since, compared to photons, neutrons posses a spin, penetrate deeper into materials, and because the neutron-scattering cross-sections can vary strongly for different isotopes of the same element, they are a much more sensitive and versatile tool.

In the tutorial the basic experiments that can be performed with neutrons, in particular neutron scattering, are described and a number of examples from material and life science are given for illustration. The tutorial also includes practical hints for the application of beam time at neutron facilities.

Tutorial CPP 1.2 Sun 16:45 HSZ 403
Reflectivity and GISAS — •Roland Steitz — Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Current problems in soft and hard matter science often require insight on the nanometer scale. In this contribution we show how surface sensitive scattering of neutrons, namely neutron reflectivity (NR) and grazing incidence small angle neutron scattering (GISANS) can be utilized to reveal details on thin films and stratified systems at solid-gas and solid-liquid interfaces. The first chapter provides a brief revision of the experimental techniques and underlying principles. Successive paragraphs deal with selected examples highlighting various aspects of experimental systems under study. Paragraph two examines polymer films at solid-gas interfaces, paragraph three addresses immobilisation of a protein at solid-liquid interfaces, paragraph four investigates the structure of the boundary of a hydrophobic polymer film and its adjacent water phase. The last two paragraphs concern laterally structured systems at interfaces and magnetic thin films, respectively.

It is noted that in particular neutrons penetrate deeply into matter, which makes them most suitable for studies of buried interfaces. In addition, investigations with neutrons benefit from the negligible impact of neutrons on the sample, i.e. there is no radiation damage, and as long as soft matter samples are considered neutrons can be used to highlight defined areas of interest by partial deuteration of the sample.

15 min. break

Tutorial CPP 1.3 Sun 17:45 HSZ 403
Neutron spectroscopy on solids — •Astrid Schneidewind — Helmholtz-Zentrum Berlin für Materialien und Energie

Neutron scattering is an outstanding and often a unique technique to study the dynamic properties of solids on an atomic scale. The tutorial will give an overview about the opportunities and the constraints of the method. Coming from the understanding of the properties of the neutron and the lattice, the nuclear and magnetic cross-sections for the interaction of the neutron with the lattice will be shown. Typical problems and the results of the required measurements will be presented and used to illustrate the aspects of the different techniques, with focus on three axis spectroscopy and time-of-flight methods. The specific role of neutron scattering in studies on magnetism will be accentuated. Finally, the complementarities to other methods as Raman and infrared spectroscopy, NMR and X-ray scattering will be pointed out.

CPP 2: Biopolymers and Biomaterials I (jointly with BP)

Time: Monday 10:30–13:00 Location: ZEU 222

Topical Talk CPP 2.1 Mon 10:30 ZEU 222
Crayfish combine amorphous and crystalline mineral to build a functional tooth structure — •Barbara Aichmayer[1], Shmuel Bentov[2,3], Ali Al-Sawalmih[1], Admir Masic[1], Paul Zaslansky[1], Peter Fratzl[1], Amir Sagi[3,4], and Amir Berman[2,4] — [1]Department of Biomaterials, Max Planck Institute of Colloids and Interfaces, 14424 Potsdam, Germany — [2]Department of Biotechnology Engineering, Ben-Gurion University of the Negev, 84105, Israel — [3]Department of Life Sciences, Ben-Gurion University of the Negev, 84105, Israel — [4]The National Institute for Biotechnology in the Negev, Israel

Various strategies allow for the formation of functional tooth structures including examples as different as the self-sharpening teeth of sea-urchins and our durable human teeth. The freshwater crayfish Cherax quadricarinatus follows a unique approach of using amorphous and crystalline minerals to build the molar extension of its mandible, which serves as an efficient grinding tool. Mechanical properties with an astonishing similarity to human teeth are achieved by the combination of an enamel-like layer of oriented fluorapatite crystals and a graded structure of chitin and amorphous mineral with an increasing phosphate/carbonate ratio. The composition and structure of the crayfish molar, measured by state of the art techniques such as Raman imaging, synchrotron X-ray diffraction and micro-CT, are related to its mechanical properties and discussed with respect to the role of the calcium phosphate, which allows for the formation of the hard, crystalline coating and also helps to stabilize the amorphous mineral.

CPP 2.2 Mon 11:00 ZEU 222
Structure-property relationships of natural silk fibers as studied by time-resolved Fourier-Transform Infrared Spectroscopy (FTIR) — •Roxana Ene[1], Periklis Papadopoulos[2], and Friedrich Kremer[1] — [1]Institüt für Experimentelle Physik I, Leipzig, Germany — [2]Max-Planck- Institut für Polymerforschung, Mainz, Germany

Polarized IR-spectroscopic and mechanical measurements are combined to analyse the conformational changes in hydrogenated and partially deuterated major ampullate spider silk of Nephila edulis[1].Crystal stress can be measured from the frequency shift of main-chain vibrations. The results show that in both states of silk a serial arrangement between the crystalline and amorphous phase dominates the nanostructure. The determination of the molecular order parameters of the different moieties proves that the amide hydrogen exchange is a selective process, taking place at the surface of β-sheet nanocrystals, implying that these regions are accessible by water[2].The mechanical properties are changing dramatically when the fiber is wet due to the fact that the pre-stress of the chains interconnecting the nanocrystals is irreversibly released. A three-component combined model of crystals in serial arrangement with amorphous chains and a fraction of chains bypassing them can describe all aforementioned states of spider silk[3]. [1] P. Papadopoulos, R. Ene, I. Weidner, F. Kremer Macromol. Rapid Commun 30,(2009). [2] R.Ene, P. Papadopoulos, F. Kremer Polymer 51,(2010) [3] R. Ene, P. Papadopoulos, F. Kremer, Soft Matter 5 (2009)

CPP 2.3 Mon 11:15 ZEU 222
Mechanical properties of fiber-fiber bonds in paper studied by atomic force microscopy — •Franz Schmied[1,4], Wolfgang Fischer[2,4], Ulrich Hirn[2,4], Robert Schennach[3,4], and Christian Teichert[1,4] — [1]Institute of Physics, University of Leoben, 8700 Leoben, Austria — [2]Institute for Paper, Pulp and Fiber Technology, Graz University of Technology, 8010 Graz, Austria — [3]Institute of Solid State Physics, Graz University of Technology, 8010 Graz, Austria — [4]CD-Laboratory for Surface Chemical and Physical Fundamentals of Paper Strength, Graz University of Technology, 8010 Graz, Austria

Paper has been used as a packaging material and for printing purposes for a long time, however a fundamental quantitative understanding for the mechanisms of paper strength has not yet been worked out. A sheet of paper is a network of individual single fibers extracted from wood. During the production cycle, these single fibers need to approach close enough to form bonds between each other. The resulting network is than called paper. Here, we present a comprehensive AFM investigation of single fibers as well as fiber-fiber bonds to achieve a deeper insight into the various mechanisms [1] that bind two single pulp fibers together. Beside morphological investigations, we present force versus distance curves to study the separation of two bonded fibers as distance and force controlled experiments. With these experiments it is possible to learn more about the mechanical properties of single fiber-fiber bonds. Supported by **Mondi** and the **Christian Doppler Research Society**, Vienna, Austria. [1] Lindström, T. et al., Proc. 13th Fundamental Research Symp, 2005.

CPP 2.4 Mon 11:30 ZEU 222

Influence of temperature on the morphology of casein micellar films — •Ezzeldin Metwalli[1], Alexander Diethert[1], Joseph Adelsberger[1], Robert Cubitt[2], Ulrich Kulozik[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany — [2]ILL, 6 rue Jules Horowitz, b.p. 156, 38042 Grenoble, France — [3]TU München, Chair for Food Proc. Eng. and Dairy Tech., 85354 Weihnstephan, Germany

Casein micelles for non-food applications such as coatings, adhesives and cosmetics are the main drive to study casein micelles structure in the thin film format. The effect of temperature on the structure of casein micelle films is investigated using grazing incidence small angle neutron scattering (GISANS). GISANS has proved sensitivity to micellar structure due to a high contrast imparted by an outer shell of D_2O on the objects [1]. At different temperatures, various average micelle sizes with large size distribution are due to an aggregation behavior of the casein proteins. For freshly prepared samples, the average micelle size is increasing from about 80 to 120 nm with increasing temperatures from 5 to 35 °C. Aged casein micelles films for 100 days at room temperature indicate a continuous structural reorganization. The continuous aggregation between hydrated micelles in the film to reach equilibrated structures explains the high stability of casein-based coatings and adhesives by the ability to adapt itself to varying environmental conditions. [1] E. Metwalli et al., Langmuir 25, 4124 (2009)

CPP 2.5 Mon 11:45 ZEU 222

Thermodynamics of chondroitin sulfate solutions using field-theoretic methodologies — •Stephan A Baeurle[1], Michael G Kiselev[2], Elena S Makarova[2], and Evgenij A Nogovitsin[2] — [1]Department of Chemistry and Pharmacy, Institute of Physical and Theoretical Chemistry, University of Regensburg, Universitätsstr. 31, D-93053 Regensburg, Germany — [2]Institute of Solution Chemistry, Russian Academy of Sciences, 153045 Ivanovo, Russia

Articular cartilage is predominantly composed of chondroitin sulfates, which are known to affect in a decisive way the mobility and flexibility of our joints. Progress in understanding their frictional-compressive behavior on the molecular level has been hindered due to the lack of reliable experimental data and the multitude of controlling parameters, influencing their structure and properties under physiological conditions. Here, we discuss the thermodynamic response of aqueous chondroitin sulfate solutions to changes in the monomer and added salt concentrations, using a recently developed field-theoretic approach beyond the mean-field level of approximation (S.A. Baeurle et al, Polymer 50, 1805-1813 (2009)). We compare our calculation results to experimental as well as molecular modeling data, and demonstrate that our field-theoretic approach provides useful estimates for important physical properties, affecting their frictional-compressive behavior.

CPP 2.6 Mon 12:00 ZEU 222

The swelling/stability effect of hyaluron on a lipid multilayer system — •Martin Kreuzer[1], Markus Strobl[2], Matthias Reinhardt[2], Reiner Dahint[1], and Roland Steitz[2] — [1]Universität Heidelberg, Physikalisch Chemisches Institut, 69120 Heidelberg, Germany — [2]Helmholtz-Zentrum Berlin GmbH, 14109 Berlin, Germany

Hyaluron (HA) is a high molecular weight polysaccharide. HA is involved in a wide range of processes in the human body, such as wound healing, severe stress, tumor progression and invasion. It was possible to show, that HA also stabilizes lipid multilayer systems at physiological conditions: Neutron reflectometry measurements, carried out at V6 and BioRef neutron reflectometer at the Helmholtz-Zentrum Berlin, in excess D2O verified, that a oligolamellar DMPC lipid bilayer coating remains stable on a silicon substrate at 21°C in its ordered state ($L\beta$) with a d-spacing of 66Å, but detaches almost completely at 38°C in its chain-disordered $L\alpha$ state from the solid support - the origin of the loss of the oligolamellar DMPC bilayer stack at 38°C is unclear. By contrast oligolamellar lipid bilayers remain stable on a substrate at 38°C when incubated with a solution of HA in D2O: In an independent experiment, an oligolamellar lipid bilayers stack was measured against a solution of 3mg/mL HA in D2O. The sample was investigated shortly after incubating at 21°C and after raising sample temperature to 38°C. The oligolamellar lipid layer remained stable on the substrate, but an immense swelling occurred until a d-spacing of 209Å is reached. We will discuss a possible mechanism of the transformation of the oligolamellar lipid system with incubation time.

CPP 2.7 Mon 12:15 ZEU 222

Influence of the intercalating fluorescent dye YOYO-1 on DNA properties — •Katrin Günther[1], Ralf Seidel[2], and Michael Mertig[1] — [1]Technische Universität Dresden, Institut für Physikalische Chemie, Mess- und Sensortechnik, 01069 Dresden, Germany — [2]Technische Universität Dresden, Biotechnology Center, Tatzberg 47-51 01307 Dresden, Germany

Fluorescent dyes of the cyanine family are widely used for staining DNA in order to explore the statistical-mechanical properties and the dynamical behaviour of DNA, even though their impact on the mechanical and structural properties has not been reliably quantified so far.

The influence of the bis-intercalating fluorescent dye YOYO-1 on the mechanical and structural properties of the molecule duplex is investigated in a wide range of staining ratios. Magnetic tweezers were used to measure the persistence and the contour length as well as the dye-induced untwisting of DNA molecules. The ionic conditions were found to considerably affect the stability of YOYO-1 binding to DNA. In contrast to other intercalating dyes, we found the persistence length remaining constant independent on the amount of bound YOYO-1.

CPP 2.8 Mon 12:30 ZEU 222

Stiffening effect of cholesterol on large unilamellar vesicles based on POPC — •Thomas Hellweg[1], Laura Rodriguez-Arriaga Rodriguez-Arriaga[2], Ivan Lopez-Montero[2], Bela Farago[3], and Francisco Monroy[2] — [1]Universität Bielefeld, PC III, Universitätsstr. 25 33615 Bielefeld, Germany — [2]Universidad Complutense, 28040 Madrid, Spain — [3]ILL, 6 rue Jules Horowitz, BP 156, F-38042 Grenoble Cedex 9, France

In the present contribution the center of mass diffusion and shape fluctuations of unilamellar POPC vesicles are studied by means of neutron spin-echo (NSE) in combination with dynamic light scattering (DLS). The intermediate scattering functions were measured for several different values of the momentum transfer q and for different cholesterol contents in the membrane. The combined analysis of NSE and DLS data allows the calculation of the bending elastic constant κ of the bilayer. A stiffening effect monitored as an increase of κ with increasing cholesterol molar ratio is evidenced from these measurements [1]. At high values of q apparently intermonolayer friction modes can be resolved using NSE [2]. The presented approach could also be applied to study the influence of membrane proteins on κ or of substances like e.g. Gramicidine.

[1] Rodriguez Arriaga, L., I. Lopez-Montero, F. Monroy, G. Orts Gil, B. Farago und T. Hellweg: Biophys. J., **96**, 3629–3637, 2009.

[2] Arriaga, L. R., R. Rodriguez-Garcia, I. Lopez-Montero, B. Farago, Th. Hellweg, und F. Monroy: Euro. Phys. J. E, **31**, 105–113, 2010.

CPP 2.9 Mon 12:45 ZEU 222

Investigation of L-Cysteine in aqueous solution using the RIXS-map approach — •Frank Meyer[1], Lothar Weinhardt[1], Monika Blum[2], Marcus Bär[3], Regan Wilks[3], Wanli Yang[4], Clemens Heske[2], and Friedrich Reinert[1] — [1]Exp. Physik VII, Universität Würzburg — [2]Department of Chemistry, University of Nevada Las Vegas, USA — [3]Solar Energy Research, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH — [4]Advanced Light Source, Lawrence Berkeley National Laboratory, USA

Amino acids are the building blocks of many biologically relevant macro-molecules. Consequently, their electronic structure is of fundamental interest and hence has been the topic of many studies. Most investigations focus on solid-state samples, the study of amino acids in their native (i.e. aqueous) environment with core-level spectroscopy has only become possible as a result of the development of specialized experimental set-ups. In combination with a high-transmission soft x-ray spectrometer, our liquid flow through cell allows us to measure two-dimensional resonant inelastic x-ray scattering (RIXS) maps of liquids and solutions. RIXS maps display the x-ray emission intensity as a function of emission and excitation energy and hence provide a comprehensive picture of the electronic structure of the investigated material. In this contribution, we will present RIXS maps of aqueous cysteine solutions at various pH values. We observe a significant impact of the pH value and evidence for proton dynamics on the time scale of the RIXS process. The results are compared to RIXS and photoemission measurements of cysteine thin films and of related molecules.

CPP 3: Interfaces and Thin Films I

Time: Monday 10:30–13:00 Location: ZEU 160

CPP 3.1 Mon 10:30 ZEU 160

Depinning of 2D Droplets in a Free Energy Model — •Daniel Herde, Stephan Herminghaus, and Martin Brinkmann — MPI for Dynamics and Self-Organization, Göttingen, Germany

While the problem of a moving contact line on an ideal substrate has been studied for some time, the dynamic behaviour on a heterogeneous substrate is not yet fully understood. Even the pinning behaviour of droplets, where they stay in place even though an external force is applied, is not characterised properly. We use a free energy approach to numerically describe the depinning of 2D droplets at single defects, on periodic and on randomly patterned substrates in the static limit.

The simulations for a single defect agree with a simple prediction for the force required for depinning, relating it to the maximum wettability contrast. Periodic substrate wettabilities lead to a set of new phenomena, as the system can display more than one stable pinned state. The determined depinning forces deviate strongly from the single pinning site case. These findings agree with our small Reynolds number fluid dynamics simulations.

CPP 3.2 Mon 10:45 ZEU 160

Order and phase behavior of cylinder forming diblock copolymers and nano-particles mixture in confinement : A Molecular Dynamics study — •Lenin Singh Shagolsem[1,2] and Jens-Uwe Sommer[1,2] — [1]Leibniz Institute of Polymer Research Dresden — [2]Institute of Theoretical Physics, TU Dresden

We study a coarse grained model of cylinder forming diblock copolymers and nano-particles mixture confined between Lennard-Jones hard walls. Both non-selective and selective nano-particles cases are considered. For non-selective nano-particles two models of interactions between monomers and nano-particles are used. Here, we focused on the role of interfaces and particles clustering, uptake and segregation of particles as a function of temperature and overall particle volume fraction, and the influence of particles on morphology. On the other hand, for the case of selective nano-particles, we systematically explored the various ordered structures formed in this restricted environment.

CPP 3.3 Mon 11:00 ZEU 160

Mechanical Properties of Random Block Copolymer Melts in the Bulk and at Selective Substrates — •Birger Steinmüller and Marcus Müller — Institut für Theoretische Physik, Georg-August-Universität, Göttingen

Random block copolymers are interesting materials to study since they show microphase separation, while lacking longer-ranged order, in a melt. We use two different coarse-grained models to access the properties of these systems via computer simulations:

The Single-Chain-in-Mean-Field simulation (SCMF), which uses a soft, density-dependent non-bonded interaction, and the Lennard-Jones bead-spring model. For the latter model we use LAMMPS, since simulating the melt via MD allows us to access the frozen state (glass) at low temperatures.

In order to determine the mechanical properties of the melt, we equilibrate the system, then quench it below the glass transition temperature. We use this glass to calculate, via a virial expansion, the local mechanical properties, e.g., local compressibility and local shear modulus. This approach is used for bulk systems, as well as for melts in contact with a selective substrate. We compare the mechanical properties of the interface and the interphase with those of the bulk. Another type of interface in the bulk, the boundary region between domains with a high concentration of the two different sorts of monomers, is additionally considered.

CPP 3.4 Mon 11:15 ZEU 160

Approach to polymer brushes of spherical monomers — •Dirk Romeis[1,2], Holger Merlitz[1,3], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung, 01069 Dresden — [2]TU Dresden, Fachbereich Physik, 01062 Dresden — [3]Department of Physics and ITPA, Xiamen University, Xiamen 361005, P. R. China

Recent experiments [1] for the creation of polymer brushes achieved considerable high grafting densities ($\sigma \geq 1/nm^2$) and subsequently chain stretchings up to $70-90\%$. In this range the behavior can no longer be approximated using the Gaussian chain model. Furthermore MD simulations [2] of brushes of densely grafted chains revealed significant instabilities of the brush surface upon slight variations of individual chains/chain ends. Analytical SCF approach for a polymer brush of spherical monomers [3] is not applicable to study these effects as it fully neglects fluctuations. We present a modified Scheutjens-Fleer method to account for a spherical shape of the monomers, compare the results with other approaches [2],[3] and give a quantitative analysis of the observed surface instabilities, which entail the behavior of a phase transition. [1] Devaux C. et. al. [*Macromolecules* **38** 4296, 2005]. [2] Merlitz H. et. al. [*Macromolecules* **41** 5070, 2008]. [3] Biesheuvel M. et. al. [*Macromolecules* **41** 6254, 2008].

CPP 3.5 Mon 11:30 ZEU 160

Ferrocene-Pyridine Block Copolymers at the Air/Water Interface and in Solution — •Martin Müller[1], Markus Gallei[2], Roland Klein[2], Bernd Stühn[1], and Matthias Rehahn[2] — [1]Institut für Festkörperphysik, 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]. Langmuir technique and in-situ X-Ray reflectivity on the water/gas interface were used to investigate the surface properties and conformations as a function of molecular weight (brush regimes and mushroomlike structures). In addition time dependent X-Ray reflectivity revealed surface structure relaxations of the pyridine blocks at the air/water interface. SAXS was used to determine structure of the PVFc-*b*-P2VP solutions. The results indicate the formation of vesicles with relative narrow size distributions. Combining the different methods leads to a detailed understanding of PVFc-P2VP structures.

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

[2] M. Gallei et al. Macromolecules, 2010, 43 (4), 1844-1854

CPP 3.6 Mon 11:45 ZEU 160

Polyoxazoline Brushes: Fabrication, Characterization and Applications — •Mukesh Agrawal[1], Juan Carlos Rueda[2], Petra Uhlmann[1], Martin Müller[1], Frank Simon[1], Carla Chung[1], and Manfred Stamm[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Strasse 6, 01069 Dresden, Germany — [2]Laboratorio de Polimeros, Sección Física, DGI, Pontificia Universidad Católica del Perú, Lima, Perú

In this study, we explore the fabrication of poly(2-isopropyl-2-oxazoline) brushes on macroscopic surfaces by exploiting the *grafting-to* approach. Firstly, carboxyl functionalized poly(2-isopropyl-2-oxazoline) molecules have been synthesized by ring opening cationic polymerization and subsequently, resulting polymer chains have been grafted onto the underlined substrates in brush-like conformation. A wide range of analytical tools including ellipsometry, contact angle, X-ray photoelectron spectroscopy, attenuated total reflection infrared spectroscopy and atomic force microscopy have been employed to characterize the polyoxazoline brushes. Finally, fabricated polymer brushes have been used to control adsorption of inorganic nanoparticles and protein molecules on macroscopic surfaces.

CPP 3.7 Mon 12:00 ZEU 160

Reversible structuring of azobenzene polymer films by surface plasmons — Tobias König and •Svetlana Santer — Department of Experimental Physics, Potsdam

Our group is interested in interactions between nano-particles and nano-structured polymer surfaces. We have shown that it is possible to move adsorbed nano-objects with relative ease, in large number and simultaneously without using external devices. The essential idea is not to put more effort in fighting against the prevailing surface forces but rather to utilize them - in clear contrast to current techniques of nano-manipulation with AFM [Santer, Adv Mat 2006]. For this, the topography should be reversible switching by changing the morphology at the scale of objects to be moved. In this work, we choose light for changing the polymer topography. Here we present azo thin films [Seki, Chem Soc Jpn 2007] with integrated optically active elements supposed to support and steer the response of polymer films to external illumination. During irradiation surface plasmon polarizations (SPP) are generated on a metallic mask. The interaction of the SPP with azo polymers results in printing of near field intensity distributions into topography with the pattern size below the diffraction limit. The topography can be driven reversible. This allows us to analyze different patterns by changing polarization or wavelength at the same position. We also examine the structuring process depending on different metallic patterns like nanogab, nanohole and hexagonal pattern. By confirmation with FDTD simulation we are able to analyze the forces which are responsible for the imprints at the azo air interface.

CPP 3.8 Mon 12:15 ZEU 160

Biomimetic crystalization of iron oxides at liquid interfaces studied by x-ray scattering experiments — •Florian Wieland[1], Patrick Degen[2], Steffen Bieder[1], Michael Paulus[1], Martin Schroer[1], Christoph Sahle[1], Johannes Möller[1], Heinz Rehage[2], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, Otto-Hahn-Str. 4, 44227 Dortmund, Germany — [2]Fakultät Chemie, Technische Universität Dortmund, Otto-Hahn-Str. 6, 44227 Dortmund, Germany

Biomineralization processes provide composite materials which show a hierarchical organization, complex and controlled shapes. In living organisms the biomineralization process is controlled by complex biological mechanisms and by the environment where the process takes place. We have investigated in-situ the mineralization of iron oxide at Langmuir monolayers at the aqueous solution-air interface. Information on the vertical density profile were obtained by x-ray reflectivity measurements where the structural evolution of the mineral layer could be observed. Furthermore grazing incidence diffraction measurements were performed in order to evaluate the crystal structure of the iron oxide and the lateral structure of the Langmuir layer. For the investigation of the local structure of the forming film surface sensitive extended x-ray absorption fine structure measurements were performed. The formation of a thin amorphous layer of iron oxide under Langmuir monolayers which posses a negative or positive headgroup was observed. The EXAFS data show that the iron coordination is similar to the coordination in maghemite, but without long range ordering.

CPP 3.9 Mon 12:30 ZEU 160

Surface templated orientation of α-helical poly(L-lysine)/polyanion complexes on unidirectionally texturised substrates — •Martin Müller[1], Wuye Ouyang[2], Thomas Keller[3], and Klaus Jandt[3] — [1]Leibniz Institute of Polymer Research (IPF) Dresden — [2]Unilever, Shanghai, P.R. China — [3]Institute of Materials Science and Technology (IMT) , University Jena

Oriented polyelectrolyte complex layers of stiff α-helical poly(L-lysine) (PLL) and poly(styrenesulfonate) (PSS) or poly(vinylsulfate) (PVS) were deposited on either unidirectionally mechanically scratched silicon substrates (i) or thin unidirectionally melt-drawn (md) poly(ethylene) (PE) films (ii) applying the layer-by-layer concept. Based on ATR-FTIR dichroism of the Amide I/II band and SFM image analysis averaged cone opening angles γ of bundled α-PLL rods in the range $\gamma = 12^\circ$ - 35° for both substrate types were found, from which high in-plane orientation was concluded. On the mechanically texturised Si substrates (i) fibrous rod-like deposits were aligned along the scratching direction and the orientation showed a significant molecular weight effect of PLL and of PSS, which can be interpreted by a topographical confinement effect of nanoscopic surface grooves on PLL/polyanion rods. Whereas, on the md-PE films (ii) fibrous rod-like deposits were aligned normal to the drawing direction, which can be interpreted by a templating effect of oriented lamellae and regular amorphous/crystalline patterns. Applications of such oriented PEL complex structures are enantiospecific surfaces for the separation of chiral drugs as well as templates for directed cell growth.

CPP 3.10 Mon 12:45 ZEU 160

Thermal tuning of micro-structured conducting polymer thin films — •Robert Meier[1], Hsin-Yin Chiang[1], Matthias A. Ruderer[1], Shuai Guo[1], Johannes Wiedersich[1], Volker Körstgens[1], Jan Perlich[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany — [2]HASYLAB at DESY, 22603 Hamburg, Germany

Conducting polymers have already shown their great potential for versatile applications such as organic light emitting diodes or thin film transistors. For such applications many routes have been invented to structure thin films on the micro- and even the nanoscale. Since conducting polymers often have a low glass transition temperature the shape of polymeric microstructures can be tuned by posterior annealing. In this work we present an in-situ grazing incidence small angle x-ray scattering study of the influence of thermal treatment on microchannels made of conducting polymers. These structures are fabricated via a new and easy fabrication routine combining a structured master and a film transfer technology. The temperature depending collapsing of the channels reveals a constant transition from sharp side walls to wavy surfaces. Such structured surfaces yield an increased light reflection and hence allow an enhanced optical absorption interesting for organic solar cells. The study is complemented with atomic force microscopy and scanning electron measurements of the polymeric microstructures before and after thermal treatment.

CPP 4: Focus Session "Nanoparticles, Nanocrystals and Colloids" (jointly with MA)

Time: Monday 10:15–13:00 Location: HSZ 103

Topical Talk CPP 4.1 Mon 10:15 HSZ 103

Magnetic nanoparticles: fundamentals and applications — •Andreas Hütten — Physics of Nanostructures, Department of Physics, Bielefeld University

Our contribution highlights recent advances in synthesis, characterization, self-assembly and sensing applications of monodisperse magnetic Co and Co based alloyed nanoparticles. A brief introduction into solution phase synthesis techniques as well as the magnetic properties and aspects of the self-assembly process of nanoparticles will be given with the emphasis placed on selected applications. Here, the presentation focuses on:- Combining magnetic nanoparticles with XMR-sensor technology - Fabrication of granular magnetoresistive sensors by employment of particles themselves as sensing layers - Employing magnetic nanoparticles as reconfigurable materials in lab-on-a-chip devices.

Topical Talk CPP 4.2 Mon 10:45 HSZ 103

Directing the Self-Assembly of Nanoparticles — •Alexander Böker — DWI an der RWTH Aachen e.V. — Lehrstuhl für Makromolekulare Materialien und Oberflächen, RWTH Aachen

This talk deals with the use of different interfaces as templates for the self-assembly of various colloidal particles. First, we describe classical oil/water emulsion systems, the so-called Pickering Emulsions. Here, the controlled nanoparticle assembly can lead to permeable, yet robust membranes and capsules. Furthermore, fluid interfaces as found in block copolymer nanostructures can be employed. Here, the nanoparticles may impart specific functions to the nanostructures, such as magnetism or charge transport as required in magnetic data storage media or polymer-based photovoltaic devices, respectively.

Moreover, we demonstrate that wrinkled polydimethylsiloxane (PDMS) substrates, with wavelengths on the order of only a few hundred nanometers, guide the assembly of rod-like tobacco mosaic virus (TMV) nanoparticles or spherical microgels. Wrinkled substrates with pre-aligned nanoparticles are used as inked stamps to transfer large particle arrays onto flat substrates. The characteristic spacing and form of the structures can be controlled by the properties of the stamp.

Topical Talk CPP 4.3 Mon 11:15 HSZ 103

Magnetic Fluids - Properties and Applications — •Stefan Odenbach — TU Dresden, Chair of Magnetofluiddynamics, 01062

Dresden

Suspensions of magnetic nanoparticles in approriate carrier liquids - so called ferrofluids - exhibit normal liquid behaviour coupled with superparamagnetic properties. The use of appropriate surfactants for the particles enables longterm stabilisation of the suspensions making them suitable for numerous technical and even medical applications.

The peculiarity of ferrofluids is given by the fact that moderate magnetic fields in the order of 10mT can significantly change the fluids properties - e.g. their viscosity - and can also provide the possibility to control the flow of such fluids.

Within the presentation a general (partly experimental) introduction of ferrofluids, their properties and applications will be followed by a discussion of magnetic flow control for biomedical applications of ferrofluids. This problem - actually discussed within the frame of novel cancer therapies - enlightens the strong interdisciplinarity of ferrofluid reserach covering fields from chemistry over physics and engineering towards medicine.

15 min. break

Invited Talk CPP 4.4 Mon 12:00 HSZ 103

Semiconductor nanocrystals — •Andrey Rogach — City University of Hong Kong

Semiconductor nanocrystals of essentially every composition can nowadays be synthesized in large quantities by inexpensive and versatile solution based approaches. They are attractive objects for use as building blocks in different functional nanostructures. We provide an overview of strongly emissive semiconductor nanocrystals synthesized in our labs and demonstrate several approaches for nanocrystals assembly. Advanced optical spectroscopy provides important insights into fundamental photophysical properties of semiconductor nanostructures. Different application aspects of functional structures based on semiconductor nanocrystals ranging from energy transfer structures to biological markers will be discussed.

Topical Talk CPP 4.5 Mon 12:30 HSZ 103

Ion and pH sensing with colloidal nanoparticles: tailoring hybrid FRET-based nanobiosensors — •Martin Oheim — Centre National de la Recherche Scientifique, CNRS UMR8154; Institut National de la Santé et de la Recherche Médicale - INSERM U603; Université Paris Descartes, Laboratory of Neurophysiology & New Microscopies

In biological cells, the free cytoplasmic ion concentration ([Ca2+]i)plays important roles in a plethora of intracellular signalling cascades. One way to attain specificity and to increase the bandwidth of Ca2+ signaling is the confinement of excursions of [Ca2+]i from baseline to micro- and nanoscale domains. Due to their ephemerous nature (nm scale, ms kinetics) the experimental detection of Ca2+ microdomains has presented a major challenge to microscopists. In my contribution I will present ongoing efforts of a franco-german-american 'nanoFRET' consortium that aims at conceptualizing, designing, validating and using novel hybrid nano-particle/organic dye-based nanobiosensors for the detection of intracellular ion-concentration nanodomains. After a swift motivation of our "pointilistic" imaging approach and the presentation of the general sensor concept, I will discuss how core/shell properties, donor-acceptor distance, stoichiometry and surface effects affect sensor performance. Preliminary sensing applications of Ca2+ and protons will be presented. I shall equally discuss the challenges for loading and imaging single-nanoparticle in live cells and ways to address these.

CPP 5: Organic Semiconductors I: Solar Cells A (jointly with HL, DS)

Time: Monday 14:00–17:30 Location: ZEU 222

Topical Talk CPP 5.1 Mon 14:00 ZEU 222

Light harvesting in single polymer chains and inorganic nanostructures — •John M. Lupton — Institut für Experimentelle und Angewandte Physik, Universität Regensburg — Department of Physics and Astronomy, University of Utah, Salt Lake City

Optimization of materials for energy conversion applications requires an understanding of intermolecular heterogeneity to ultimately formulate synthetic approaches to maximizing the fraction of a particular subensemble. Single molecule spectroscopy can offer such insight as an exquisitely sensitive tool to unravel the underlying complexity of organic semiconductors. In the context of solar cells, for example, the technique can help to identify purely intramolecular exciton migration and charge separation processes.

Recently, we have explored the migration of excitons in single molecules as a function of the initial excitation energy, thus offering information on thermalization processes within the polymer chain. The approach allows a direct spectroscopic identification of the absorption of individual chromophores on the chain, whereas mere emission tends to provide information only on the lowest-energy unit in the intramolecular excitonic cascade [1].

The heterogeneity in light-harvesting characteristics is particularly pronounced in semiconductor nanostructures, where particle morphology directly influences the heterojunction band structure and the excitonic spectrum [2].

[1]Walter et al., Phys. Rev. Lett. 103, 167401 (2009).

[2]Borys et al., Science (in press).

CPP 5.2 Mon 14:30 ZEU 222

Highly efficient vacuum processed BHJ solar cell based on merocyanines — •Vera Steinmann[1], Hannah Bürckstümmer[2], Nils M. Kronenberg[1], Martin R. Lenze[1], Dirk Hertel[1], Frank Würthner[2], and Klaus Meerholz[1] — [1]Department für Chemie, Universität Köln, Germany — [2]Institut für Organische Chemie and Röntgen Research Center for Complex Material Systems Universität Würzburg, Germany

Bulk heterojunction (BHJ) organic solar cells have attracted considerable interest due to their potential for large-scale, cost-effective and environmentally friendly power generation. Small molecules have been successfully introduced in solution- (SOL) as well as vacuum- (VAC) processed devices, reporting efficiencies (PCE) up to 4.4% and 5.7% respectively. For simple layer stack devices (2-3 layers) based on CuPc as electron donor and C60 as electron acceptor PCEs up to 5.0% have been achieved.

Recently, we presented a direct comparison of highly efficient SOL and VAC BHJ cells based on merocyanine dyes (MC) with a similarly simple layer stack as reported in the literature. Our most efficient devices exhibited PCEs up to 4.9%. Further optimizations on the VAC processed cells led to high PCEs exceeding 6% while keeping the same simple layer stack. In addition, these cells have demonstrated exceptional performance even at lower light intensities.

Due to the simple chemical variability of MC dyes, they are ideally suited for tandem solar cells. We will present first attempts in this direction.

CPP 5.3 Mon 14:45 ZEU 222

Efficiency-Limiting Processes in Bulk Heterojunction Organic Solar Cells — Ian Howard, Ralf Mauer, Fabian Etzold, Valentin Kamm, Michael Meister, Hannah Mangold, and •Frédéric Laquai — Max Planck Research Group for Organic Optoelectronics, MPI for Polymer Research, Mainz, Germany

Despite significant study, the efficiency-limiting processes that govern the efficiency of bulk heterojunction photovoltaic devices still remain ambiguous. In particular the role of interfacial charge-transfer (CT) states as potential intermediates of free charge carriers is diversely debated. In this contribution we directly observe charge generation and recombination processes in state-of-the-art polymer:methanofullerene photovoltaic blends by transient absorption spectroscopy and compare polythiophene (P3HT) of varying regioregularity and low-bandgap polymers as electron donor materials. We observe a common feature of these blends is ultrafast (< 100 fs) exciton dissociation at the donor-acceptor interface. However, a certain fraction of excitons create CT states that predominantly recombine geminately within a few nanoseconds. On the other hand the fraction of free charge carriers recombines bimolecularly on a time scale competing with charge extraction and can thus be swept out of the device as photocurrent. The results demonstrate the importance of ultrafast free carrier generation and suppression of interfacial CT state formation to achieve high power conversion efficiencies in various material systems. [1] I.A. Howard, R.

Mauer, M. Meister, F. Laquai, J. Am. Chem. Soc. 2010, 132, 14866. [2] I.A. Howard, F. Laquai, Macromol. Chem. Phys. 2010, 211, 2063.

CPP 5.4 Mon 15:00 ZEU 222

Bias-Dependent Transient Absorption on Organic Solar Cells; Connection to Device Performance?

— •Ian Howard, Ralf Mauer, Valentin Kam, Michael Meister, and Frédéric Laquai — Max Planck Forschungsgruppe für Organische Optoelektronik, Max-Planck-Institut für Polymerforschung, Mainz, Deutschland

We directly observe the bias dependence of charge-transfer state separation in organic bulk heterojunctions using in-situ transient absorption on operating organic solar cells. The effect of bias on charge-transfer state lifetime ($<$ 2ns) is found to be minimal, however suppression of nongeminate recombination with bias on later timescales ($>$10 ns) is observed and explains the bias dependence of the photocurrent. The bias independence of charge-transfer state separation is directly applicable to interpreting organic solar cell performance under standard AM1.5 illumination. However, due to the differences in charge densities and dynamic versus steady-state behavior between pulsed measurements and standard operating conditions, the effects of bias on the suppression of nongeminate recombination are not simplistically transferable. We consider to what extent pulsed transient absorbtion techniques on devices can be used to reveal nongeminate recombination mechanisms in devices operating under standard illumination conditions.

CPP 5.5 Mon 15:15 ZEU 222

Degradation effects related to the hole transport layer in organic solar cells

— •Bernhard Ecker[1], Jairo Nolasco[2], Josep Pallarés[2], Lluis Marsal[2], Jörg Posdorfer[3], Jürgen Parisi[1], and Elizabeth von Hauff[1] — [1]Energy and Semiconductor Research Laboratory, Institute of Physics, Carl von Ossietzky University, 26111 Oldenburg (Germany) — [2]Departament d'Enginyeria Electrònica Elèctrica i Automàtica, Universitat Rovira i Virgili, Avda. Països Catalans 26, 43007 Tarragona (Spain) — [3]Enthone Nano Science Centre, Ormecon GmbH, Ferdinand-Harten-Str. 7, 22949, Ammersbek (Germany)

We discuss the influence of the hole transport layer on the device stability in organic bulk-heterojunction solar cells. Two water based hole transport layers, poly(3,4-ethylenedioxythiophene) : poly(styrene sulfonate) (PEDOT:PSS) and polyaniline : poly(styrene sulfonate) (PANI:PSS), and one isopropyl alcohol based PANI:PSS transport layer were investigated. Solar cells were prepared with the three different hole transport layers and degraded under illumination. Current-voltage, capacitance-voltage, and capacitance-frequency data were collected at varying light intensities over a period of 7 hours. Solar cell performance and stability were compared between non encapsulated and encapsulated samples to obtain understanding about degradation effects related to oxygen and water as well as degradation mechanisms related to the intrinsic instability of the solar cell materials and interfaces. We show that the properties of the hole transport layer can have a significant impact on the stability of organic solar cells.

15 min. break

CPP 5.6 Mon 15:45 ZEU 222

Characterization of trap states in small-molecule organic solar cells by using Impedance Spectrocopy.

— •Lorenzo Burtone, Debdutta Ray, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden Germany

In this work, we focus on the characterization of trap levels in the electronic gap of organic semiconductors used in solar cells. These states can modify the electric field inside the device, considerably affecting charge generation and transport and consequently the solar cell efficiency. A method to characterize traps by using impedance spectroscopy is presented. We propose a new equivalent circuit based on previously reported theoretical models and we apply it in the fitting procedure of the measured data. In particular, we measure the impedance spectra of two flat heterojunction small molecule solar cells, where one of them has doped electron and hole transport layers. We observe the contribution of trap states at low frequencies in the capacitance spectra for the devices with doped transport layers. The experimental results can be understood with the equivalent circuit proposed and the trap state contribution can be evaluated. From a fitting procedure, we estimate the density of trap states to be around $1\text{x}10^{17}\text{cm}^{-3}\text{eV}^{-1}$. Moreover we observe from the impedance analysis the presence of dopants in the intrisic layer with an estimated effective concentration of about $8.4\text{x}10^{17}\text{cm}^{-3}$. This value is in agreement with very low doping concentration and suggests the formation of a non-abrupt junction between intrinsic and doped layers.

CPP 5.7 Mon 16:00 ZEU 222

The effect of energetic disorder on open-circuit voltage in organic photovoltaics

— •James C Blakesley, Ilja Lange, and Dieter Neher — University of Potsdam, Germany

Open-circuit voltage (VOC) is one of the most important figures of merit describing the quality of organic photovoltaics (OPVs). Usually it is assumed that VOC depends on the energy difference between the highest occupied molecular orbital (HOMO) of the donor and the lowest unoccupied molecular orbital (LUMO) of the acceptor, but large deviations from this trend are often found. In reality, there is a distribution of energy levels within the components, and this should also be taken into account.

We simulate bulk heterojunction OPVs using a simulation that includes the effects of energetic disorder [1].We find that VOC depends on: 1) the nominal donor-HOMO to acceptor-LUMO energy gap; 2) the charge-carrier generation and recombination rates; 3) the electrodes; and 4) the amount of energetic disorder. While the first three of these points have been much discussed previously, the effect of the fourth has not been conclusively demonstrated. An increase in the amount of energetic disorder leads to a reduction in the VOC due to relaxation of the carriers into the lowest lying energy levels. We find an analytical expression that predicts well the modelled VOC, and suggest the use of an effective donor-acceptor energy gap that takes energetic disorder into account. Measurements of Fermi-level pinning might be useful for determining this effective energy gap. [1] J. C. Blakesley and N. C. Greenham, J. Appl. Phys. 106, 034507 (2009)

CPP 5.8 Mon 16:15 ZEU 222

Modelling Temperature-Dependent Current-Voltage Curves of Organic Photovoltaic Devices

— •Simon Züfle, Martin T. Neukom, Benjamin Perucco, Nils A. Reinke, and Beat Ruhstaller — ICP, ZHAW, Winterthur, Schweiz

Current-voltage curves allow to determine both fill-factor and efficiency of organic photovoltaic devices and are therefore a commonly used characterisation technique. Since analytical models for current-voltage curves fail in describing the fundamental processes of photogenerated current, more complex numerical calculations are mandatory for obtaining insight into the device physics. The analysis of multiple current-voltage curves at different temperatures calls for CPU-efficient algorithms combining state-of-the-art physical models and high calculation speed.

In order to model current-voltage curves simple drift-diffusion calculations with constant mobilities and thermionic emission as injection model are frequently used. In this study we investigate current-voltage curves measured at different temperatures with the help of a nonlinear least-square fitting algorithm in combination with a comprehensive physical model for charge carrier transport and injection. We evaluate the performance of different models for charge carrier transport, including the Gaussian Disorder Model, by simultaneously fitting multiple curves and discussing the mathematical quality of the fit. We employ an efficient algorithm for extracting material-specific parameters that allows modelling of measured current-voltage curves on a minute time-frame with a desktop PC.

CPP 5.9 Mon 16:30 ZEU 222

Role of drift and diffusion in organic solar cells measured by transient photocurrents

— •Wolfgang Tress, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, TU Dresden, Dresden, Germany

The role of the electric field and the contribution of diffusion to photocurrents are controversially discussed in the case of organic solar cells. We investigate flat heterojunction organic solar cells with systematically varied barriers at the contacts that are created by a HOMO offset between donor and hole transport layer. These barriers lead to S-kinks in the IV curve and to strong imbalanced and even reversed forces on charge carriers resulting from the field on the one hand and the concentration gradient on the other hand. By applying a rectangular illumination signal with varied light intensities, we observe in the photocurrent transients a pile-up of charge carriers at an extraction barrier. If an injection barrier is present, there exists a region in the IV curve where charges are extracted against the electric field by a strong diffusion gradient. These findings are based on the analysis of transient current data in the μs regime using electrical simulations based on a drift-diffusion model. The simulations show that observed overshoots in the photocurrent transients result from these imbalance effects and give new insights into the working principle of organic solar cells.

CPP 5.10 Mon 16:45 ZEU 222

Charge extraction with linearly increasing voltage: A numerical model for parameter extraction — •Martin Neukom, Simon Züfle, Nils Reinke, and Beat Ruhstaller — Institute of Computational Physics, Technikumstr 9, 8401 Winterthur, Switzerland

Device characterisation is an essential part in the process of improving the performance and lifetime of organic solar cells. Most of the device and material parameters are not accessible by measurements therefore sophisticated measurement techniques in combination with numerical simulations are needed to extract these parameters. A frequently used method to determine material parameters like charge carrier mobilities and the recombination coefficient is the CELIV technique (charge extraction by linearly increasing voltage). In this technique a voltage ramp is applied to the device in order to extract free charge carriers inside the bulk. With a simple analytical formula the mobility is commonly estimated on the basis of the temporal position of the current peak. We simulate the CELIV experiment, transient and steady-state measurement techniques with a fully-coupled opto-electronic model. On the one hand we investigate the limitations of the analytical formulas for mobility determination. On the other hand we use our model to fit several experimental datasets simultaneously to obtain elementary material parameters like the electron and hole mobility, recombination coefficient, photon to charge conversion efficiency and injection barriers in both printed and spin-coated bulk heterojunction solar cells. We deduce the influence of these material parameters on the overall device performance.

CPP 5.11 Mon 17:00 ZEU 222

Simulating electron transfer reactions in organic solar cell components — •Harald Oberhofer[1] and Jochen Blumberger[2] — [1]Department of Chemistry, University of Cambridge, UK — [2]Department of Physics and Astronomy, University College London, UK

Organic solar cells are envisaged as a promising alternative to silicon based solar cells. They are cheap and easy to produce, light and flexible, and easily deployed on walls or roofs. Unfortunately, these advantages currently come at the price of small photo-electric conversion efficiencies. To help overcome this deficiency we use advanced density functional theory (DFT) based methods to investigate the electron-conducting properties of modified Fullerene crystals which are commonly used as electron-conducting component in organic solar cells.

In our contribution we will briefly discuss the techniques used to estimate electron transfer rates from computer simulations. Then we present our calculations on modified Fullerene crystals. We studied $C_{61}H_2$—a commonly used test system—and [6,6]-phenyl-C61-butyricacid-methyl-ester (PCBM) for 3 different crystal lattices which are commonly found in experiments. In the crystal we estimated electron transfer rates between next- and next-nearest neighbours with and without the application of an external electric field. These results where then used to estimate the electron mobility for the different lattice types. These results can represent a starting point for the optimisation of electron conduction in next-generation organic solar cells.

CPP 5.12 Mon 17:15 ZEU 222

Time resolved microwave conductivity reveals charge carrier dynamics in organic semiconductors — •Johannes Erben[1], Andreas Sperlich[1], Hannes Kraus[1], Tom J. Savenije[1,3], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius-Maximilians-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 organic semiconductors is essential to improve material properties and processing parameters, and, at long sight, device performance. Time Resolved Microwave Conductivity (TRMC) gives direct access to the microscopic transport properties, as the high frequency alternating electric field limits the drift of the charge carriers. After laser pulse excitation TRMC signal decays in P3HT:PCBM blends with varying PCBM content have been observed exhibiting a power law time dependence. The influence of morphology and temperature on the charge carrier recombination and mobility on a microscopic scale can thus be investigated.

CPP 6: Charged Soft Matter

Time: Monday 14:00–17:30 Location: ZEU 160

CPP 6.1 Mon 14:00 ZEU 160

Charge transport and glassy dynamics in confined neat and polymerized ionic liquids — •Joshua Sangoro, Ciprian Iacob, Wycliffe Kipnusu, and Friedrich Kremer — Institute of Experimental Physics I, University of Leipzig, Leipzig, Germany

Charge transport and glassy dynamics in neat and polymerized ionic liquids under one- and two- dimensional confinement are investigated in a wide frequency and temperature ranges by a combination of Broadband Dielectric Spectroscopy (BDS) and Pulsed Field Gradient Nuclear Magnetic Resonance (PFG NMR) [1-2]. By applying the Einstein-Smoluchowski relations to the dielectric spectra, diffusion coefficients are obtained in quantitative agreement with independent PFG NMR. The impact of geometrical confinement as well as the pore wall-ionic liquid interactions on the overall ionic mobility is explored for diverse categories of ionic liquids. The results are discussed within the framework of glassy dynamics assisted charge transport in ionic liquids.

References

[1] Iacob, C., Sangoro, J. R., Papadopoulos, P., Schubert, T., Naumov, S., Valluilin, R., Kärger, J. and Kremer, F. (2010). Phys. Chem. Chem. Phys., 12, 13798-13803.

[2] Sangoro, J. R., Iacob, C., Serghei, A., Friedrich, C., and Kremer, F. (2009) Phys. Chem. Chem. Phys., 11 (5) 913; Krause, C., Sangoro, J.R., Iacob, C. and Kremer, F. (2010) J. Phys. Chem. B, 114, 382-386; Sangoro, J.R., Iacob, C., Serghei, A., Naumov, S., Galvosas, P., Kärger, J., Wespe, C., Bordusa, F., Stoppa, A., Hunger, J., Buchner, R., and Kremer, F. (2008) J. Chem. Phys., 128 (21) 214509.

CPP 6.2 Mon 14:15 ZEU 160

Vapour pressure of ionic liquids — •Markus Bier — Max-Planck-Institut f. Metallforschung, Stuttgart, Germany

The probably most exciting property of room temperature ionic liquids (RTILs), i.e. molten salts with melting temperatures below 100 C, is their extraordinary low vapour pressure at the triple point. It is shown how this feature can be understood on the basis of a simple thermodynamic argument. It will become clear why the tiny triple point pressures are a common feature of RTILs and it is argued that RTILs are the only class of liquids which are expected to exhibit such low vapour pressures.

[1] M. Bier and S. Dietrich, Mol. Phys. 108, 211 (2010).

[2] M. Bier and S. Dietrich, Mol. Phys. 108, 1413 (2010).

[3] M. Bier and S. Dietrich, arXiv:1006.2090v1.

CPP 6.3 Mon 14:30 ZEU 160

Theoretical Reconstruction of Photoelectron-Spectra for Imidazolium-Based Ionic Liquids — •Wichard J. D. Beenken, Markus Reinmöller, Julia Preiss, Jelena Pajovic, Angela Ulbrich, Stefan Krischok, and Erich Runge — Institute of Physics and Institute of Micro- and Nanotechnologies, Ilmenau University of Technology, P.O. Box 100 565, 98684 Ilmenau, Germany

We have previously measured valence-band XPS, UPS and MIES spectra of room-temperature ionic liquids formed by bis(trifluoromethylsulfonyl)imide anions ($[Tf_2N]^-$) and 1-ethyl-3-methyl-imidazolium ($[EMIm]^+$) and 1-octyl-3-methyl-imidazolium ($[OMIm]^+$) cations [1]. In the present work, we demonstrate how to reconstruct these XPS/UPS spectra in terms of orbital-specific partial densities of states (pDOS), which are calculated by density functional theory (DFT), and XPS/UPS cross-sections known from literature. This method allows us to identify not only the stoichiometry of the ionic liquid, but also to attribute spectral features to specific chemical positions within the ions. Furthermore, we extend this method to the analysis of MIES-spectra. Since the surface-sensitivity increases from XPS over UPS to MIES, we do not only obtain depth profiles for the stoichiometry but our analysis provides even information about the orientation of the ions at the ionic-liquid surface.

[1] Ikari, T.; Keppler, A.; Reinmöller, M.; Beenken, W. J. D.; Krischok, S.; Marschewski, M.; Maus-Friedrichs, W.; Höfft, O.; Endres, F. e-J. Surf. Sci. Nanotech. 2010, 8, 241.

CPP 6.4 Mon 14:45 ZEU 160

Systematic Analysis of the Surface Structure of Ionic Liquids using Sum Frequency Generation (SFG) — •Markus Reinmöller[1,2], Chariz Peñalber[2], Gabriela Adamová[3], Kenneth R. Seddon[3], and Steven Baldelli[2] — [1]Ilmenau University of Technology, Institute for Physics, Weimarer Straße 32, D-98693 Ilmenau, Germany — [2]University of Houston, Department of Chemistry, 136 Fleming Building, Houston, TX 77204-5003, USA — [3]Queen's University Belfast, QUILL Research Centre, David Keir Building, Stranmillis Road, Belfast, BT9 5AG, Northern Ireland (UK)

The surface structure (surface composition and orientation) of phosphonium-based ionic liquids in the system $[P_{888x}][Cl]$ is studied under systematic variation of the length of one alkyl chain (x = 4, 5, 8, 10, 12, and 14) by SFG. The nonlinear optical method of sum frequency generation vibrational spectroscopy (SFG) obtains its surface sensitivity due to the requirement of the broken centro-symmetry, which is present at surfaces and interfaces [1]. Vibrations of both CH_2- and CH_3-groups from the alkyl chains of the $[P_{888x}]^+$ ion are observed. For this type of phosphonium-based ionic liquids a model for the surface structure will be proposed [2].

Additionally we have performed quantum-chemical calculations using density functional theory (DFT), as demonstrated recently [3].

[1] R. Lu, et al., J. Phys. Chem. B, 108 (2004) 7297. P. B. Miranda, et al., J. Phys. Chem. B, 103 (1999) 3292. [2] C. S. Santos, et al., Chem. Soc. Rev., 39 (2010) 2136. [3] T. Ikari, et al., e-J. Surf. Sci. Nanotech., 8 (2010) 241.

CPP 6.5 Mon 15:00 ZEU 160

Novel Concept for Reporting Pressure - fields based on Mechanoresponsive Polyelectrolyte Brushes — •Johann Erath[1], Johanna Bünsow[2], Wilhelm T. S. Huck[2,3], and Andreas Fery[1] — [1]Physical Chemistry II, University Bayreuth, 95440, Bayreuth, Germany — [2]Melville Laboratory for Polymer Synthesis, Department of Chemistry, University of Cambridge, Cambridge CB21EW, UK — [3]Radboud University Nijmegen, Institute for Molecules and Materials, 6525 AJ Nijmegen, The Netherlands

Determination of pressure fields is of interest for both, fundamental science (e.g. mapping force fields in bio-adhesion) and application (e.g. robotics). The aim of this contribution is to introduce a novel concept for self-reporting force sensors based on mechanoresponsive polyelectrolyte brushes, which translate deformation directly into changes in fluorescence intensity. Experiments were performed with a combination of an atomic force microscope with a confocal laser scanning microscope. Using the soft colloidal probe technique, we compressed the polyelectrolyte brushes in the direction normal to the surface. Compression leads to a drop of the fluorescence intensity in the brush. Likewise, upon retracting the bead from the surface, a tension was exerted onto the polymer strands situated at the edge of the bead which induced an increase of the fluorescence signal. The response of the polyelectrolyte brushes to compression was completely reversible. On the basis of the JKR theory, we developed a qualitative understanding of the force distribution underneath the PDMS bead, which shows that the sensor does response to compression and tension in one frame.

CPP 6.6 Mon 15:15 ZEU 160

Optimization of ionic force fields based on ion-pair thermodynamic properties — •Maria Fyta, Immanuel Kalcher, Joachim Dzubiella, and Roland Netz — Physics Department, Technical University of Munich, 85748 Garching

We investigate strategies to optimize ionic force fields based on single-ion and ion-pair properties simultaneously. To that end, we present results using Molecular Dynamics simulations for five different salt solutions, namely CsCl, KCl, NaI, KF, and CsI, at finite ion concentration. The force fields of these ions are systematically varied under the constraint that the single-ion solvation free energy matches the experimental value, which reduces the two-dimensional $\{\sigma, \varepsilon\}$ parameter space of the Lennard Jones interaction to a one dimensional curve. From the finite-concentration simulations, the pair-potential is extracted and the osmotic coefficient is calculated, which is compared to experimental data. A strong dependence of the osmotic coefficient on the force field is evident, which is remarkable as the single-ion solvation free energy and the ion-water structure remain invariant under the parameter variation. Optimization of the force field is achieved for the cations Cs$^+$ and K^+, while for the anions I$^-$ and F$^-$ the experimental osmotic coefficient cannot be reached. We suggest, thus, that additional parameters might have to be introduced into the modeling, for example by modified mixing rules and present data along these lines.

15 min. break

Topical Talk CPP 6.7 Mon 15:45 ZEU 160

Charge-Controlled Protein Crystallization — •Fajun Zhang[1], Georg Zocher[2], Andrea Sauter[1], Marcell Wolf[1], Felix Roosen-Runge[1], Thilo Stehle[2,3], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Germany — [2]Institute for Biochemistry, University of Tübingen, Germany — [3]Department of Pediatrics, Vanderbilt University School of Medicine, Nashville, Tennessee, USA

We have studied the phase behavior of model globular proteins in solution in the presence of multivalent counterions. Under these conditions, it has been shown that negatively charged globular proteins undergo a reentrant condensation (RC) phase behavior [1], i.e. a phase-separated regime occurs in between two critical salt concentrations, c* < c**, giving a meta-stable liquid-liquid phase separation (LLPS). This RC phase behavior corresponds to an effective charge inversion of proteins as confirmed by zeta-potential measurements and supported by Monte Carlo simulations [2]. Crystallization near phase boundaries follows different mechanisms. Close to c*, crystal growth follows classical nucleation and growth mechanism; close to c**, crystallization follows a meta-stable LLPS, namely a two-step mechanism. X-ray diffraction analysis of the high quality single crystals provides direct evidence of crystal structure and cation binding sites. Our discovery of RC and LLPS induced by multivalent cations provides a new way to tune protein interactions with predictable phase behavior as well as controlling protein crystallization. [1] F. Zhang, et al., Phys. Rev. Lett. 2008, 101, 148101. [2] F. Zhang, et al., Proteins, 2010, 78, 3450

CPP 6.8 Mon 16:15 ZEU 160

Formation of complexes between linear and spherical polyelectrolytes — Ute Böhme and •Ulrich Scheler — Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden

Pulsed-field-gradient (PFG) NMR is a versatile tool for the investigation of the hydrodynamic size of molecules and small complexes in solution. In combination with electrophoresis NMR it permits the determination of the effective charge free of any model. PAMAM dendrimers are used as example for spherical weak polyelectrolytes. Their nominal charge is adjusted by the pH-dependent protonation of the amin groups. The protonation is monitored via the chemical shift of adjacent CH2 protons. The effective charge of the PAMAM dendrimers is significantly lower than the nominal charge, which is determined from the protonation of the amino groups. With increasing generation of the dendrimers an increasing fraction of counterions condenses up to 75%. Poly(styrene sulfonate) has been used as a linear strong polyelectrolyte to study the formation of complexes between linear and spherical polyelectrolytes. The fraction of poly(styrene sulfonate), that binds to the dendrimers increases with increasing effective charge of the dendrimer, which is observed in both diffusion and electrophoresis NMR.

CPP 6.9 Mon 16:30 ZEU 160

Selective Adsorption of Spherical Polyelectrolyte Brushes onto Polyelectrolyte Multilayers — •Christoph Hanske[1], Alexander Wittemann[2], and Andreas Fery[1] — [1]Department of Physical Chemistry II, University of Bayreuth, Germany — [2]Department of Physical Chemistry I, University of Bayreuth, Germany

Ordered mesostructures of functional colloids are promising building blocks for future lab-on-a-chip devices such as sensors. The production of these materials requires precise control over the effective particle-substrate interactions. Here we discuss the electrosteric interaction between polyelectrolyte multilayers and spherical polyelectrolyte brushes (SPB). These colloids consist of a glassy core and a stimuli-responsive layer of densely grafted polyelectrolyte chains. The polyelectrolyte brush allows tuning the shape of the particles in solution as well as adjusting their adsorption behavior in the presence of charged surfaces. Kinetic studies at low ionic strength reveal rapid SPB adsorption on oppositely charged substrates, whereas equally charged surfaces efficiently prevent colloidal attachment. This marked selectivity results from the particle morphology and can be explained in terms of counterion release and electrosteric repulsion. The extent of particle adsorption depends sensitively on electrostatic screening. With increasing ionic strength, the equilibrium surface coverage is raised on both types of substrate at the expense of selectivity. Accounting for this parameter, we were able to assemble two-dimensional arrays of SPB utilizing chemically patterned substrates.

CPP 6.10 Mon 16:45 ZEU 160

Anomalous small angle X-ray scattering studies of multivalent cations binding and distribution in protein 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

Charge-induced protein-protein interactions attract much attention due to their direct relation to protein crystallization and protein association related diseases. For the interaction of proteins by multivalent cations, which shows a re-entrant condensation phase behavior, the distribution of cations is crucial [1]. So far, anomalous Small Angle X-Ray Scattering (ASAXS) has provided the best way to study this issue by selecting the energies away and near the absorption edge of the target ions [2]. Here we studied protein solutions in the presence of YCl_3 in the re-entrant regime. The ASAXS experiments were performed at the ESRF using 12 different energies near the K-absorption edge of yttrium. Systematic measurements of Y^{3+} around the proteins show clearly visible ASAXS shifts in the scattered intensity. The pure resonant signal for the multivalent ion has been successfully separated using the matrix method. These data can prove vital for modeling protein-cation interactions and the mechanisms of the protein re-entrant condensation behavior. The results will be discussed with regard to the binding number and distribution of Y^{3+} within the diffusion zone. [1] F. Zhang, et al. Phys. Rev. Lett. 2008, 101, 148101. [2] M. Sztucki, et al. J. Appl. Cryst. 2010, 43, 1479.

CPP 6.11 Mon 17:00 ZEU 160

Reversed Hofmeister Series: The Interplay of Surface Charge and Surface Polarity — •Nadine Schwierz — Physik Department, Technische Universitaet Muenchen, James Franck Strasse, 85748 Garching, Germany

More than 120 years ago, Hofmeister discovered that different ions can be ordered reproducibly according to their efficiency in precipitating hen-egg white proteins. That sequence now runs under the name Hofmeister series and can be found everywhere in chemistry and biology. The complex interplay of electrostatics, dispersion forces, hydration, ion size effects and interfacial water structure make it hard to identify a universal law. We describe a two-scale modeling approach toward anion specificity at surfaces of varying charge and polarity. Explicit-solvent atomistic molecular dynamics simulations at neutral hydrophobic (nonpolar) and neutral hydrophilic (polar) self-assembled monolayers furnish potentials of mean force for sodium and the halide anions, which are then used within Poisson-Boltzmann theory to calculate ionic distributions at surfaces of arbitrary charge for finite ion concentration. We obtain the direct anionic Hofmeister series at negatively charged hydrophobic surfaces. Reversal takes place when going to negative polar or to positive nonpolar surfaces, leading to the indirect series, while for positive polar surfaces the direct series is again obtained in full accordance with a recent experimental classification. A schematic Hofmeister phase diagram is proposed. Partial series reversal is understood as a transient phenomenon for surfaces of intermediate polarity or charge.

CPP 6.12 Mon 17:15 ZEU 160

Simulations of charged dendrimers with flexible spacer-chains and explicit counterions — •Jaroslaw Sylwester Kłos[1,3] and Jens-Uwe Sommer[1,2] — [1]Leibniz Institute of Polymer Research Dresden, Germany — [2]Institut for Theoretical Physics, TU Dresden, Germany — [3]Faculty of Physics, UAM Poznan, Poland

We study the properties of weak dendritic polyelectrolytes with flexible spacer-chains of various lengths and explicit counterions in an athermal solvent using Monte Carlo simulations based on the bond fluctuation model. The calculations are performed for molecules under neutral and low pH conditions. In the first case solely the terminal groups of the dendrimers are protonated, whereas in the second both the terminal groups and branching units are. In our approach the full Coulomb potential and the excluded volume interactions are taken into account with the reduced temperature τ as the main control parameter. Our simulations show an interplay of counterion condensation, trapping of counterions inside the dendrimer's volume and counterion evaporation into the solution which give rise to a non-monotonous electrostatic swelling of the molecule with τ. Decreasing pH leads to higher swelling and stronger spacer-length dependence. To explain the swelling effect we apply a Flory-type argument where both trapped but non-condensed counterions and uncompensated charges due to counterion evaporation are included. This model properly reflects the swelling behavior with respect to temperature, pH and spacer-length variation, though quantitatively underestimates it. We also investigate the pH-effects on density and charge profiles of the dendrimer.

CPP 7: Interfaces and Thin Films II

Time: Monday 14:00–17:30 Location: ZEU 114

CPP 7.1 Mon 14:00 ZEU 114

Cracking in thin polymer films promoted through physical ageing — •Mithun Chowdhury[1], Christophe Calers[1], Arnold Chang-Mou Yang[3], Ullrich Steiner[2,4], and Günter Reiter[1,2] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, 79104, Freiburg, Germany — [2]Freiburg Institute for Advanced Studies (FRIAS) — [3]Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, Taiwan — [4]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK

Dynamics of polymers in ultrathin films is a long standing yet ever stimulating topic in the arena of polymer physics. Being inspired by occasionally observed cracking of such films during spin-coating, we performed systematic studies on the influence of film preparation and physical ageing at temperatures close but below the glass transition. We observed the growth of cracks after ageing and cooling the films to room temperature. Hierarchical patterns of interconnecting cracks were formed. AFM inspection showed nano/micro-structures of voids and fibrils within the cracks, indicating plastic deformation similar to crazing. We tentatively suggest that physical ageing of such films causes segmental relaxations of non-equilibrated polymer chains, introducing a gradient in lateral tension within the film in the direction normal to the film surface. Considering the possibility of generating strong mechanical tension at the film surface due to the formation of a 'crust' during film preparation, we may have to consider two antagonistic origins for crack growth: gradients in stresses induced by film preparation and amplification of such gradients during physical ageing.

CPP 7.2 Mon 14:15 ZEU 114

Free volume and aging in polymers of intrinsic microporosity (PIM) — •Stephan Harms[1], Klaus Rätzke[1], Franz Faupel[1], Werner Egger[2], Luca Ravelli[2], Nhamo Chaukura[3], and Peter Budd[3] — [1]Christian-Albrechts University at Kiel, Institute for Materials Science - Multicomponent Materials, 24143 Kiel — [2]University of Armed Forces, 85577 Neubiberg — [3]University of Manchester, Manchester M13 9PL, UK

Recently developed polymers of intrinsic microporosity (PIM) are suitable candidates as state-of the art gas separation membranes. However, as thin films, like other high free volume polymers, they can undergo aging which means that permeability and free volume become time-dependent and are reduced after prolonged storing and operation time. To investigate the time dependence of free volume, positron annihilation lifetime spectroscopy (PALS) at the pulsed low energy positron system (PLEPS) at FRM II has been performed. The PLEPS setup allows the measurement of depth profiles of the free volume for thin film samples. PIM films of different thickness and preparation method were investigated at two aging times. For all samples we could detect a time dependent decrease of the free volume compare to the bulk reference value. Samples with thickness ≥ 1300 nm do not show a homogeneous reduction of free volume but a steep gradient to the surface of the film. These experiments give valuable information for understanding aging phenomena in high free volume materials.

CPP 7.3 Mon 14:30 ZEU 114

The Young's Modulus of Polyelectrolyte Multilayer: Influence of Charge Density and Ambient Water Vapours — •Ralf Köhler[1,2], Ingo Dönch[3], Patrick Ott[4], André Laschewski[4], and Andreas Fery[5] — [1]TU Berlin, Dept. Applied Physical Chemistry, 10623 Berlin — [2]HZB Berlin, Dept. Soft Matter, 14109 Berlin — [3]Max Planck Institute of Colloids and Interfaces, Dept. Interfaces, 14424 Potsdam — [4]University of Potsdam, Applied Polymer Chemistry, 14476 Potsdam — [5]University of Bayreuth, Physial Chemistry II, 95440 Bayreuth: Germany

Polyelectrolyte Multilayers (PEM) are polymer films, self-assembled by consecutive adsorption of oppositely charged polyions. Our study addresses the impact of the internal interactions in the PEM on the macroscopic mechanical behavior. The strategy is to vary the ionic interactions by using polycations of different charge densities (ChD). Furthermore the internal interactions are modified by changing the water content in the PEM by a systematic variation of the ambient relative humidity (RH). PEM of sub-micrometer thickness are prepared in Layer-by-Layer spraying technique on flexible sheets of silicone-rubber. The used polyions are PSS and PDADMAC-derivatives of different ChD. The E-modules are determined with the SIEBIMM-method. We obtained E-Moduli in the range from 0.3 to ca 1.5MPa. Basically for a higher-ChD PEM the E-Modulus is higher. But with increasing RH the PEMs soften until their E-Moduli coincide. Apparently the ionic interactions rule the mechanics in the first place but the incorporated water is able to moderate the E-Moduli over a wide range.

CPP 7.4 Mon 14:45 ZEU 114

Supported Polyelectrolyte Multilayer under Mechanical Stress: Sequential Change of the Internal Structure — •Johannes Früh[1], Adrian Rühm[2], Helmuth Möhwald[1], Rumen Krastev[3], and Ralf Köhler[4,5] — [1]MPI of Colloids and Interfaces, Dept. Interfaces, 14424 Potsdam — [2]MPI for Metal Research at FRM-2, 85747 Garching — [3]NMI at the University of Tübingen, 72770 Reutlingen — [4]TU Berlin, Dept. Chemistry: Applied Physical Chemistry, 10623 Berlin — [5]HZB Berlin, Dept. Soft Matter, 14109 Berlin. Germany

Polyelectrolyte Multilayer (PEM) are composite materials build-up of alternating layers of organic polyions of opposite charge. We study the changes of the internal structure of mechanically loaded PEM on molecular level. The PEM are prepared in layer-by-layer technique on solid substrates using PSS and PDADMAC as polyions. Small elongations ($\epsilon<0.2\%$) are studied with neutron and X-ray reflectivity on deformed PEM-coated glass slides. We observe an increase of the film thickness upon stretching. This might be a result of a formation of *molecular cavities* in the PEM. Large elongations (ϵ˜10%) are investigated with fluorescence spectroscopy on Pyrene-labelled PEM on silicone-rubber substrates. An irreversible molecular decoiling is observed upon stretching. When the limit of plastic deformation is exceeded, i.e. almost full decoiling, macroscopic cracks appear, indicating the destruction limit of the PEM. Our Study on the molecular response on external mechanical stress allows for new insights into internal processes in PEM, e.g. molecular decoiling and the creation of defects.

CPP 7.5 Mon 15:00 ZEU 114

Interdiffusion in Polyelectrolyte Multilayers during Film Formation — •Olaf Soltwedel[1], Oxana Ivanova[1], Peter Nestler[1], Ralf Köhler[2,3], and Christiane A. Helm[1] — [1]Inst. für Physik, Uni Greifswald, Felix-Hausdorff-Str. 6, D-17487 Greifswald — [2]Helmholtz-Zentrum für Materialien und Energien, Hahn-Meitner-Platz 1, D-14109 Berlin — [3]Stranski-Laboratorium für Physikalische und Theoretische Chemie, TU Berlin, Strasse des 17. Juni 112, D-10623 Berlin

Using neutron reflectivity, the internal structure of polyelectrolyte multilayers is described on the nanoscale. The polyanion is poly(styrenesulfonate) (PSS), and the polycation is poly(allylamine hydrochloride) (PAH) or poly(diallyldimethylammonium chloride) (PDADMAC). Each film consists of a protonated and a deuterated block, built from x protonated and y deuterated polycation/polyanion bilayers, respectively. The number of bilayers N = x + y is kept constant; the position of the interface between the blocks is varied systematically. The internal roughness is smallest next to the film/air interface and increases with the number of bilayers away from the film/air interface until an equilibrium value is reached. For PDAMAC/PSS films, the diffusion constant increases with the PDADMAC polymer length, therefore the interdiffusion is attributed to stress relaxation during deposition. The equilibrium internal roughness increases with PDADMAC polymer length and the salt concentration in the deposition solution. However, the number of polyanion/polycation layer pairs necessary to achieve the equilibrium internal roughness depends nonmonotonically on the salt concentration.

CPP 7.6 Mon 15:15 ZEU 114

The structure of the liquid-liquid water-CO_2 interface during hydrate formation — •Julia Nase[1], Felix Lehmkühler[2], Michael Paulus[1], Lars Böwer[1], Sebastian Tiemeyer[1], Sebastian Holz[1], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund — [2]DESY, Hasylab, 22607 Hamburg

Hydrates are ice-like inclusion compounds with gaseous guest molecules in water cages. In recent years, they have incited the interest of researchers due to both their importance in oil industry (pipeline blockage) and as a promising possibility for CO_2 sequestration. Despite the increased interest, the formation process on a molecular level is still poorly understood. MD simulations predict the existence of different pre-structures, but an experimental proof is still pendant. Hydrate formation is generally thought to be initiated at interfaces. We report on a x-ray reflectivity study of the liquid-liquid water-CO_2 interface. This technique was shown to be a reliable tool to determine the thickness and roughness of interfaces and thin layers.

Previous studies on the liquid-gas interface in the theoretical hydrate stability region could not confirm the existence of precursor structures, however, a macroscopic hydrate phase did not occur. In our present study, the high offer in CO_2 molecules at the liquid-liquid interface resulted in a macroscopic hydrate formation. Results on the roughness of this interface beyond the stability region, an information that has been lacking so far, and on structural changes just before the appearance of a macroscopic hydrate phase are presented in this talk.

15 min. break

CPP 7.7 Mon 15:45 ZEU 114

Dynamics of complex systems in the proximity of a solid interface — •Sulivan D.B. Vianna[1], Markus A. Plum[1], Hatice Duran[1,2], Hans-Jürgen Butt[1], and Werner Steffen[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]TOBB Economy and Technology University 43, 06560 Ankara, Turkey

An experimental investigation of the effect of solid surfaces (e.g Au) on the motion of colloids and dynamics of polymers is reported. The novel experimental approach for probing the interphase in a system close to the solid interface is the use of surface plasmons or optical waveguide modes as incident fields in resonance enhanced dynamic light scattering (REDLS) or waveguide enhanced dynamic light scattering (WEDLS). Our incident fields are localized at the surface. For surface plasmons the penetration depth is typically 200 nm and for the waveguides the penetration depth can be tuned typically from 100 to 1000 nm. The influence of a nearby interface on translational and rotational diffusion of colloids in solution is explored. Due to the localization and hence strong enhancement of the field in the surface plasmon or the evanescent part of the waveguides utilized, we are able to study ultrathin polymer films, i.e. dynamic processes above the glass transition.

CPP 7.8 Mon 16:00 ZEU 114

Characterization of spectral diffusion and its application to probe thin polymer films — •Daniela Täuber[1], Stefan Krause[1], Beatriz Aráoz[2], Pedro F. Aramendía[2], and Christian von Borczyskowski[1] — [1]nanoMA, TU-Chemnitz, Institut für Physik, Germany — [2]FCEN, Universidad Buenos Aires, Argentina

Dye molecules with a large solvent shift are used to probe local properties in thin polymer films. Upon excitation with the 488 nm line of an Argon-ion-laser, the emission spectra show spectral diffusion: small temporal fluctuations and larger jumps. In analogy to anomalous spatial diffusion we use a newly developed tool[1] to characterize this spectral diffusion: Probability distributions of spectral diffusivities

[2].

This method is applied to analyze different thin poly-n-alkyl methacrylate films on Si wafers with 100 nm SiOx.

[1] M. Bauer, M. Heidernätsch, D. Täuber, C. von Borczyskowski, and G. Radons, Diffusion Fundamentals, 11, 2009, 104.

[2] S. Krause, P.F. Aramendía, D. Täuber, C. von Borczyskowski, Freezing Single Molecule Dynamics on Interfaces and in Polymers, PCCP, accepted.

CPP 7.9 Mon 16:15 ZEU 114

Measuring the Elasticity of Polymer Films with AFM Nanoindentation — •Cagri Üzüm, Anna Burmistrova, Marcel Richter, Johannes Hellwig, Dmitry Volodkin, and Regine v. Klitzing — Stranski-Laboratorium, Institut für Chemie, TU Berlin, Strasse des 17.Juni 124, 10623 Berlin, Germany

Mechanical properties of polymeric films and microparticles have to be revealed once they are to be used in biological applications [1]. For submicron structures, the (visco)elasticity can be measured by means of AFM nanoindentation. Together with its nanoscale imaging ability, this makes the AFM a unique technique in the relevant area.

In this contribution, elastic properties (Young's modulus) of poly(L-lysine)/hyaluronan (PLL/HA) thin films as well as other hydrogel films/particles were investigated. Young's modulus was observed to depend strongly on the temperature and the cross-linker density while the film thickness itself had only a minor effect. Either colloidal probes or blunt tips were used as nanoindenters. The well-known problem of determining the exact indenter-sample contact point was tried to be overcome by various data handling processes [2].

[1] Picart, C., Senger, B., Sengupta, K., Dubreuil, F., Fery, A. Colloids Surf., A 303, 30-36 (2007)

[2] Dimitriadis, E.K., Horkay, F., Maresca, J., Kachar, B., Chadwick, R.S. Biophys. J. 82, 2798 (2002)

CPP 7.10 Mon 16:30 ZEU 114

Microcantilever sensors for monitoring microdrop evaporation of pure liquids and binary mixtures — •Elmar Bonaccurso^1 and Chuanjun Liu^{1,2} — ^{1}Center of Smart Interfaces, TU-Darmstadt, Germany — ^{2}Max Planck Institute for Polymer Research, Mainz, Germany

We describe in detail a nonimaging technique [1] that allows the measurement of the mass, the radius, and the contact angle of evaporating sessile microdrops of pure liquids and binary mixtures. The microdrops were deposited onto hydrophobized silicon microcantilevers whose bending and resonance frequency were monitored during drop evaporation. We verify the laws of evaporation kinetics for microdrops with diameters from 80 down to 10 um.

The evaporation of mixtures of water/ethanol drops confirmed previous results with millimeter sized drops. N,N-dimethylformamide drops undergo a transformation from an initial spherical shape to a thin film. Flattening of the drop causes a slowdown of the evaporation kinetics at the end. Two concurring factors are at its origin: the rising disjoining pressure stabilizes the thin liquid film and the increasing radius of curvature of the drop reduces the vapor pressure [2].

[1] Bonaccurso E., Butt, H.-J., J. Phys. Chem. B 109, 253 (2005).
[2] Liu C.J. & Bonaccurso E., Rev. Sci. Instrum. 81, 013702 (2010).

CPP 7.11 Mon 16:45 ZEU 114

Laser-assisted atom probe tomography of polyelectrolyte multilayers — •Andreas Stoffers and Guido Schmitz — Institut für Materialphysik, Westf. Wilhelms-Universität, Wilhelm-Klemm-Strasse 10, 48149 Münster, Germany

Atom probe tomography (APT) is a well established tool for analyzing metals at an atomic scale. In order to explore the possibilities of analyzing polymer materials by Pulsed-laser atom probe tomography (PLAP), we have chosen the model case of polyelectrolyte multilayers (PEM). PEMs are adsorbed step by step as a multilayer of poly-anions and poly-cations at the apex of sharp gold tips. This self-assembly is driven by electrostatic forces, where every adsorbed layer induces a charge inversion of the surface. Macroscopic charge neutrality requires an exact 1:1 stoichiometry of polycation and polyanion charges or the presence of counterions within the layer. The presence of counterions in PEMs is controversially discussed and laser-assisted atom probe tomography seems to be an ideal tool to answer this question. By means of laser-assistance it is indeed possible to chemically analyze multilayers of poly(acrylic acid), poly(diallyl dimethyl-ammonium chloride), poly(styrene sulfonate) and poly(allylamine hydrochloride). In all cases the mass spectra are complex, characterized by peaks of multiple fractions of different molecular mass. Different polymer-types might be distinguished based on the intensity ratio between characteristic mass peaks. The proven amount of counterions is obviously negligible. In addition, a 3D reconstruction of a self assembled monolayer (1H,1H,2H,2H-Perfluorodecanethiol) will be presented.

CPP 7.12 Mon 17:00 ZEU 114

Phosphocholine Monolayer Solidification due to Oxygen Radicals — •Andreas Gröning^{1,2}, Heiko Ahrens^1, Thomas Ortmann^1, Frank Lawrenz^1, Gerald Brezesinski^3, Fritz Scholz^2, and Christiane A. Helm^1 — ^{1}Inst. für Physik, Uni Greifswald, Felix-Hausdorff-Str. 6, D-17487 Greifswald — ^{2}Inst. für Biochemie, Uni Greifswald, Felix-Hausdorff-Str. 4, D-17487 Greifswald — ^{3}MPI KGF, D-14476 Potsdam

The reaction of 1,2-dipalmitoylphosphatidylcholine (DPPC) with hydroxyl-radicals has been investigated using monolayer techniques: isotherms, infrared absorption reflection spectroscopy (IRRAS), gracing incidence X-ray diffraction (GIXD), X-ray reflection and fluorescence microscopy. The DPPC monolayer undergoes a transition from a liquid-expanded to a liquid-condensed state characterized by a plateau region. The DPPC monolayer is attacked in the coexistence region and in the liquid-condensed state with different Fenton concentrations. With increasing Fenton concentration, the plateau region is shifted to a lower surface pressure; eventually it disappears. With higher Fenton concentration, the molecular area in the liquid-condensed phase is decreased. IRRAS experiments indicate a decomposition of the choline group. After Fenton attack, GIXD shows a decrease of the tilt angle, an increase of translational (by 50%) and orientational order which demonstrates monolayer solidification. The highly compressed monolayer exhibits nearly hexagonal order. Additionally, fluorescence microscopy shows that some DPPC domains fuse and new domains nucleate. At zero pressure, solid domains remain.

CPP 7.13 Mon 17:15 ZEU 114

Effect of oppositely charged hydrophobic additives (alkanoates) on the stability of C_{14}TAB foam films — •Natascha Schelero^1, Reinhard Miller^2, and Regine von Klitzing^1 — ^{1}Stranski-Laboratorium, Department of Chemistry, TU Berlin, Strasse des 17. Juni 124, 10623 Berlin — ^{2}Max Planck Institute of Colloids and Interfaces, Am Mühlenberg 1, 14424 Potsdam

Liquid foams are frequently applied in daily life and industrial processes (e.g. cleaning agents, personal care products and fire-fightening). In most of the applications mixtures of several components are used. Model systems for such applications are thin liquid films. Within this work the impact of the hydrophobicity of oppositely charged additives on the stability of C_{14}TAB foam films are investigated. Furthermore, the surface properties of the mixed systems are described to gain a general understanding about the surface characteristics. Since C_{14}TAB and alkanoates are oppositely charged, the question arises whether charge reversal at the film surfaces occurs and how it depends on the chain length of the alkanoate.

CPP 8: Poster: Organic Semiconductors

Time: Monday 17:30–19:30 Location: P2

CPP 8.1 Mon 17:30 P2

Spectroscopic Signatures of Anions on C60, C70 and C80 — •Moritz Liedtke^{1,2}, Carsten Deibel^2, and Vladimir Dyakonov^{1,2} — ^{1}Energy Technology, Bavarian Centre for Applied Energy Research (ZAE Bayern), 97074 Würzburg, Germany — ^{2}Experimental Physics VI, Julius-Maximilian University of Würzburg, 97074 Würzburg, Germany

We applied photo-induced absorption technique to find the signatures of electrons on fullerenes in polymer:fullerene blends used for organic photovoltaic and pure fullerene layers. These negative charge carriers show different excitation energies into higher states which seem to depend only on the fullerene size and not on the sidechains of the fullerenes or the polymer used. The knowledge of these signatures might offer new insights in the process of charge carrier generation by exciting only the polymer in the blend while probing the electron on the fullerene.

CPP 8.2 Mon 17:30 P2

Temperature dependant investigation of charge-transfer states in P3HT:PC60BM studied by time resolved ESR — •Magdalena Zawadzki[1], Andreas Sperlich[1], Hannes Kraus[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, D-97074 Würzburg

The time resolved ESR-technique (trESR) is a powerfull tool to study the temporal evolution of charge-transfer states (CTS) photogenerated at the donor-acceptor interface. Right after the photoexcitation, spin-polarized radical pairs are formed in the system, showing themselves as an alternating pattern of microwave absorption and stimulated microwave emission (A/E/A/E). At longer timescales the pattern converts into pure absorption one (A/A) due to free charges in the blend. The separation dynamics within the pair as well as the thermalization are assumed to be dependent on the temperature. In this contribution, we report on temperature dependent trESR studies performed on thin films of P3HT:PCBM bulk-heterojunction.

CPP 8.3 Mon 17:30 P2

Morphology and electronic triplet states of regioregular P3HT and PCPDTBT ultrathin films — •Stefan Väth[1], Hannes Kraus[1], Andreas Sperlich[1], Mario Zerson[2], Robert Magerle[2], Carsten Deibel[1], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University Würzburg, D-97074 Würzburg — [2]Chemische Physik, TU Chemnitz, D-09107 Chemnitz — [3]ZAE Bayern, Div. Functional Materials for Energy Technology, D-97074 Würzburg

The intensively studied donor polythiophene P3HT and the novel low band-gap donor-acceptor copolymer PCPDTBT are used in very well performing solution processed organic solar cells. Therefore, understanding the materials' electronic properties and in particular the influence of morphology on them is crucial for optimizing the device preparation as well as the synthesis of novel organic semiconductors. We gain access to the morphological bearing on the triplet state employing angle resolved optically detected magnetic resonance (ODMR) on very thin ordered films, a technique sensitive to the alignment of exciton triplet states. Furthermore we attempt to link these results with high resolution Nanotomography images of the film morphology.

CPP 8.4 Mon 17:30 P2

Multifrequency LESR of P3HT:C70 blends — •Johannes Römer[1], Andreas Sperlich[1], Hannes Kraus[1], Oleg Poluektov[2], Carsten Deibel[1], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — [2]Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL 60439, USA — [3]ZAE Bayern, D-97074 Würzburg

For application in polymer bulk heterojunction solar cells, the blend of the polythiophene P3HT and the $PC_{70}BM$ fullerene electron acceptor material is a promising model system, as C_{70}-derivatives are used in the most efficient organic solar cells.

Using high-frequency electron spin resonance (ESR), we were able to separate the signals of the positive polaron from the negative anion localized on the C_{70}-cage, and the involved g-tensor components could be obtained. The focus of this work is the analysis of the main parameters of light induced ESR spectra obtained at different microwave frequencies, namely 9, 36, and 130 GHz.

CPP 8.5 Mon 17:30 P2

Investigation of recombination process in organic bulk heterojunction solar cells — •Jędrzej Szmytkowski — University of Saskatchewan, Saskatoon, Canada — Gdańsk University of Technology, Gdańsk, Poland

The mechanism of charge carrier recombination in organic solar cells is still under debate. Although Langevin model of bimolecular recombination is usually used with success, the experimental deviations from this theory have been observed. Recently, several different scenarios have been proposed for explanation. To make further progress, we have analyzed recombination coefficient as a function of several physical parameters. The obtained good agreement between theoretical and experimental results is promising.

CPP 8.6 Mon 17:30 P2

Effect of Nongeminate Recombination on Fill Factor in Polythiophene:Methanofullerene Organic Solar Cells — •Ralf Mauer, Ian A. Howard, and Frédéric Laquai — Max Planck Institute for Polymer Research, Mainz, Germany

A key factor in solar cell efficiency is the dependence of the photocurrent on applied bias. With respect to organic solar cells, it is often suggested that this factor is governed by the field dependence of charge-transfer state separation. Here we demonstrate that this is not the case in benchmark polythiophene:methanofullerene solar cells. By examining the temperature and light intensity dependence of the current voltage characteristics we determine that: 1) the majority of free charge generation is not dependent on temperature, and 2) the competition between extraction and recombination of free charges principally determines the dependence of photocurrent on bias. These results are confirmed by direct observation of the temperature dependence of charge separation and recombination using transient absorption spectroscopy and highlight that in order to achieve optimal fill factors in organic solar cells minimizing free carrier recombination is an important consideration.

CPP 8.7 Mon 17:30 P2

Charge Generation and Recombination in PCDTBT:PCBM Photovoltaic Blends — •Fabian Etzold, Ian Howard, Ralf Mauer, Michael Meister, and Frédéric Laquai — Max Planck Institute for Polymer Research, Mainz, Germany

Low-bandgap donor-acceptor copolymers have recently demonstrated their potential in bulk heterojunction organic solar cells. Among them, poly[N-9'-heptadecanyl-2,7-carbazole-alt-5,5-(4',7'-di-2-thienyl-2',1',3'-benzothiadiazole)] (PCDTBT) blended with fullerene derivatives proved to be very efficient, yielding power conversion efficiencies in excess of 3 % even without postproduction annealing, which is typically applied to polythiophene:fullerene blends. We investigate exciton dynamics in pristine PCDTBT and charge carrier dynamics in as-cast and annealed blends with [6,6]-phenyl C_{61} butyric acid methyl ester (PCBM) by transient absorption and time-resolved photoluminescence spectroscopy. We find that in PCDTBT:PCBM blends a large fraction of excitons undergoes ultrafast generation of free charge carriers as previously observed for other material systems including P3HT:PCBM. However, a fraction of interfacial charge transfer states is also created, which recombine geminately with a lifetime of 2.5 ns. By monitoring the recombination dynamics over the previously unobserved time range from 1 ns to 1 ms, we conclude that the device efficiency must be limited by geminate recombination and charge extraction.

CPP 8.8 Mon 17:30 P2

Morphological and Photophysical Characterisation of Novel Absorber Materials for Organic Solar Cells — •Hannah Mangold[1], Silvia Janietz[2], Ingo Lieberwirth[1], Michael Meister[1], Ian H. Howard[1], and Frédéric Laquai[1] — [1]Max-Planck-Institut für Polymerforschung, Mainz, Germany — [2]Fraunhofer Institut für Angewandte Polymerforschung, Potsdam, Germany

In this contribution new tailor-made fluorene based terpolymers are investigated as absorber materials in organic solar cells. These terpolymers contain different contents of dialkyl-substituted diphenylbenzopyrazine or diphenyl-thienopyrazine and triphenylamine units and possess bandgaps between 1.3 and 1.8 eV. Power conversion efficiencies up to 3% with open circuit voltages close to 1 V are obtained in blends with [6,6]-phenyl C61 butyric acid methyl ester (PCBM) even without prior thermal treatment. The morphology of the blends is investigated by atomic force microscopy (AFM) and transmission electron microscopy (TEM) and correlated with the results obtained from I-V-measurements under simulated sunlight. Photophysical experiments such as steady-state photoinduced absorption (PIA) and transient absorption (TA) spectroscopy are employed to understand the effect of variation of the polymer structure on exciton dissociation and charge recombination. Using a combination of these methods the understanding of the structure-property-relationship of these materials is extended towards the molecular scale and the impact of molecular structure and processing conditions on charge generation, transport and recombination processes can be elucidated.

CPP 8.9 Mon 17:30 P2

Effects of 1,8-Diiodooctane and 1,8-Octanedithiol on the performance of low bandgap devices — •Vida Turkovic[2], Sebastian Engmann[2], Miguel Carrasco-Orozco[1], Harald Hoppe[2], and Gerhard Gobsch[2] — [1]Merck Chemicals Ltd. Chilworth Technical Centre, University Parkway, Southampton SO16 7QD, UK — [2]Technisches Universitaet Ilmenau, Fakultaet fuer Mathematik und Naturwissenschaften, Institut fuer Physik, Experimentalphysik I, Weimarer Strasse 32, 98693 Ilmenau

We have tested the role of octanedithiol (ODT) and diiodooctane (DIO) on the performance of organic solar cells. They are known to contribute in improving the performance of the lowbandgap polymer PCPDTBT devices. We investigated their influence on the performance of other novel low bandgap polymers. Different amounts of ODT and DIO were added to different low bandgap polymer/PC70BM blend systems. Optical, morphological and electrical properties of solar cells are reported.

CPP 8.10 Mon 17:30 P2

Targeted Side Chain Substitution for Tuning the Photovoltaic Performance of Conjugated Polymers — •S. Rathgeber[1], D. Bastos de Toledo[2], F. Kühnlenz[3], R. Jadhav[3], G. Adam[4], H. Hoppe[3], and D.A.M. Egbe[4] — [1]Johannes-Gutenberg-University Mainz, Institute for Physics, Mainz — [2]MPI Mainz, Polymer Physics, Mainz — [3]TU Ilmenau, Institute for Physics, Ilmenau — [4]Linz Institute for Organic Solar Cells, Johannes-Kepler-University Linz, Austria

We used targeted side chain (SC) substitution for tuning the performance of poly(arylene-ethynylene)-alt-poly(arylene-vinylene) (PAE-PAV) copolymers in polymer:PCBM bulk heterojunction (BHJ) solar cells. The layered structure (degree of order, inter-layer- and pipi-stacking distance) was systematically modified by linear alkyloxy- and/or branched 2-ethylhexyloxy SC substitution. We identified a correlation between polymer architecture, structural properties as investigated by x-ray scattering techniques, photophysical characteristics and photovoltaic performance in the device. Optimization led to a statistical copolymer, comprising linear and branched SC statistically distributed along the backbone. This material combines the benefits of linear- and branched-substituted polymers i.e. high supramolecular order in combination with good solubility at low volume fraction of isolating SC. It exhibits high charge carrier mobilities and high power conversion efficiencies of 3.8% in BHJ solar cells - the present state-of-the-art value for PAV-based materials. We consider this approach to be transferable to other material classes. (Macromolecules 2010, 43, 306; Macromolecules 2010, 43, 1261; J. Mater. Chem. 2010, 20, 9726)

CPP 8.11 Mon 17:30 P2

Effect of annealing processes on morphology of photoactive polymer layers for solar cell applications — •Weijia Wang, Matthias A. Ruderer, and Peter Müller-Buschbaum — TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany

The interest in photoactive polymers and its applications in organic photovoltaics increased in the last decades dramatically. The promise of these materials for production of mechanical stable, light weight and easy processible organic solar cells at low cost make them especially interesting. Currently the major drawback is still the low efficiencies compared to standard inorganic solar cells and the short lifetime. It was found that morphology plays an important role in both areas. Therefore the importance of structure control is crucial. We investigated the influence of different control parameters such as annealing and blending ratio on a bulk heterojunction systems based on a polythiophene derivative. The changes in structure were monitored with imaging methods such as AFM. The effect on molecular level is investigated by absorption and photoluminescence measurements.

CPP 8.12 Mon 17:30 P2

Solution Processed Organic Bulk Heterojunction Tandem Solar Cells — •Steve Albrecht and Dieter Neher — Soft matter Physics, University of Potsdam, D-14476 Potsdam, Germany

One of the critical issues regarding the preparation of organic tandem solar cells from solution is the central recombination contact. This contact should be highly transparent and conductive to provide high recombination currents. Moreover it should protect the 1st subcell from the solution processing of the 2nd subcell. Here, we present a systematic study of various recombination contacts in organic bulk heterojunction tandem solar cells made from blends of different polymers with PCBM. We compare solution processed recombination contacts fabricated from metal-oxides (TiO_2 and ZnO) and PEDOT:PSS with evaporated recombination contacts made from thin metal layers and molybdenum-oxide. The solar cell characteristics as well as the morphology of the contacts measured by AFM and SEM are illustrated. To compare the electrical properties of the varying contacts we show measurements on single carrier devices for different contact-structures. Alongside we present the results of optical modeling of the subcells and the complete tandem device and relate these results to experimental absorption and reflection spectra of the same structures. Based on these studies, layer thicknesses were adjusted for optimum current matching and device performance.

CPP 8.13 Mon 17:30 P2

Charge Transfer Processes in Hybrid Solar Cells Composed of Amorphous Silicon and Organic Materials — •Sebastian Schaefer[1], Tim Schulze[2], Lars Korte[2], and Dieter Neher[1] — [1]Universität Potsdam, Inst. Physik u. Astronomie, Karl-Liebknecht-Strasse 24/25, 14467 Potsdam-Golm, Germany — [2]Helmholtz Zentrum Berlin, Inst. für Silizium Photovoltaik, Kekuléstrasse 5, 12489 Berlin, Germany

The efficiency of hybrid solar cells composed of organic materials and amorphous hydrogenated silicon (a-Si:H) strongly depends upon the efficiency of charge transfer processes at the inorganic-organic interface. We investigated the performance of devices comprising an ITO/a-Si:H(n-type)/a-Si:H(intrinsic)/organic/metal multilayer structure and using two different organic components: zinc phthalocyanine (ZnPc) and poly(3-hexylthiophene) (P3HT). The results show higher power conversion- and quantum efficiencies for the P3HT based cells, compared to ZnPc. This can be explained by larger energy-level offset at the interface between the organic layer and a-Si:H, which facilitates hole transfer from occupied states in the valence band tail to the HOMO of the organic material and additionally promotes exciton splitting. The performance of the a-Si:H/P3HT cells can be further improved by treatment of the amorphous silicon surface with hydrofluoric acid (HF) and p-type doping of P3HT with F4TCNQ. The improved cells reached maximum power conversion efficiencies of 1%.

CPP 8.14 Mon 17:30 P2

Photophysical Study on Core-Enlarged-Rylendiimides and -Anhydrides for Dye Sensitized Solar Cells — •Belinda Nölscher, Michael Meister, Ian Howard, Glauco Battagliarin, Chen Li, Klaus Müllen, and Frédéric Laquai — Max Planck Institute for Polymer Research, Mainz, Germany

Dye Sensitized Solar Cells (DSSCs) are promising devices for lightweight and cheap photovoltaic energy conversion. Up to now many different dyes have been synthesized to improve the efficiency of these solar cells. Investigation of the relation between the photophysical properties of the dyes and their performance in solar cells is required for a better understanding of the working principle of DSSCs.

In this contribution we present a photophysical study on novel core-enlarged-rylenediimides and -anhydrides [1]. By changing the core size or expanding the bay-position the absorption maximum can be tuned and further shifted into the red part of the solar spectrum. We employ transient and steady-state photoinduced absorption as well as time-resolved photoluminescence spectroscopy to investigate the dynamics of charge generation and recombination of these dyes in solid-state DSSCs. Theoretically a higher efficiency of core-enlarged dyes due to increased photon harvesting can be expected, however, it appears that these dyes follow a different trend. Based on our results we draw conclusions for future material development of higher efficiency all-organic dyes for DSSCs.

[1] Synthesis and application of core-enlarged perylene dyes, Y. Avlasevich, C. Li, K. Müllen, Journal of Materials Chemistry

CPP 8.15 Mon 17:30 P2

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

All-organic sensitizer molecules are interesting alternatives to replace the commonly used expensive Ru-complex dyes in dye-sensitized solar cells (DSC). Dyes with large extinction coeffcients are especially interesting for solid state DSCs, which work better with thinner mesoporous TiO_2 structures. Perylene derivatives have attracted strong interest, since they combine a strong absorption with reasonably good device efficiencies if used with Spiro-MeOTAD as solid state hole transporter [1]. Here we present a photophysical study of perylene monoimide dyes (PMI) for DSCs with different functional groups attached to the core that influence the position of the HOMO and LUMO. By employing quasi steady-state photoinduced absorption spectroscopy and transient absorption spectroscopy on device-like structures, we gain insight into the mechanisms of charge generation and recombination. For instance, we found that a rise of the LUMO energy, which should in principle facilitate electron injection into the TiO_2, does not necessarily lead to more efficient charge separation. Our investigations aim to a thorough understanding of the structure-property-relationship of these PMI-based organic dyes in solid state DSCs.

1. Cappel, U.B., et al., J. Phys. Chem. C, 2009. 113(33): p. 14595-14597.

CPP 8.16 Mon 17:30 P2

Influence of different exciton blocking layers on device characteristics and solar cell degradation in a planar heterojunction DIP/C_{60} solar cell — •Christoph Schuhmair, Julia Wagner, Mark Gruber, Andreas Opitz, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

The application of exciton blocking layers (EBLs) in organic solar cells has become a well-established method to prevent exciton quenching at the acceptor/cathode interface. One of the most common exciton blocking materials is the organic semiconducting material bathocuproine (BCP), yet its precise working mechanism is not fully understood.

In this contribution we show the impact of two different EBLs (BCP and 1,4,5,8-Naphthalene-tetracarboxylic-dianhydride (NTCDA)) on the performance of planar heterojunction organic solar cells based on the donor diindenoperylene (DIP) and the fullerene C_{60} as acceptor. The studies cover the influence of the EBL thickness and its impact on device degradation. Moreover, it is shown how substrate heating during deposition of the donor material influences the growth morphology of the donor and subsequent layers leading to distinct differences in device degradation.

CPP 8.17 Mon 17:30 P2

Design of a chamber for production and *in-situ* characterization of small-molecule photovoltaic cells — •Giovanni Ligorio, Simeon Lange, Christopher Lorch, Jens Reinhardt, Alexander Hinderhofer, Alexander Gerlach, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen

The design and construction of an integrated ultra-high vacuum system to produce and characterize organic small-molecule solar cells is presented. Through the new system, it is possible to produce several solar cells simultaneously on the same ITO substrate via organic molecular beam deposition under vacuum conditions. *In-situ* electric contact is achieved through aluminum deposition. With the sample holder the temperature can be systematically modified between 200 K and 700 K while liquid nitrogen cooling or resistive heating to control the deposition process and to permit temperature dependent measurements.

We present first results for OPV cells of diindenoperylene (DIP)/C_{60} (see Ref. [1] for complementary results) and DIP/perfluoropentacene (PFP).

[1] Wagner, J., *et al.*, Adv. Funct. Mater., doi: 10.1002/adfm.201001028

CPP 8.18 Mon 17:30 P2

Automatisierte elektrische und spektrale Charakterisierung organischer Solarzellenproben — •André Merten, Ronny Timmreck, Moritz Riede und Karl Leo — IAPP/TU-Dresden, George-Bähr-Straße 1,01069 Dresden

Organische Solarzellen basierend auf kleinen Molekülen stellen eine vielversprechende Möglichkeit für eine künftige kostengünstige Versorgung mit elektrischer Energie dar. Dazu muss jedoch deren Effizienz, welche für die besten Laborzellen mittlerweile bei 8,3% liegt noch erheblich gesteigert werden. Dies geschieht vor allem durch die Suche nach neuen Absorber und Transportmaterialien sowie Untersuchung des Einfluss der Morphologie. Dies erfordert systematische Variation des Stackaufbaus hinsichtlich Material, Schichtdicke und Dotierung sowie der Prozessierungsparameter und führt zu einer hohen Zahl zu charakterisierender Proben. Hoher Durchsatz, Genauigkeit und Zuverlässigkeit erfordert eine Automatisierung der elektrischen und spektralen Charakterisierung. Die dazu am Institut für Angewandte Photophysik entwickelten und eingesetzten Instrumente zur automatischen Charakterisierung von bis zu 144 Proben werden vorgestellt und an Beispielen demonstriert. Besondere Schwerpunkt sind dabei die Korrektur des Spektralen Mismatches, die Messung der spektralen Response von Einfach- und Tandemzellen, sowie die Bestimmung der Internen Quanteneffizienz unter Berücksichtigung von gemessener EQE, Absorption sowie simulierter Absorption der aktiven Schichten.

CPP 8.19 Mon 17:30 P2

Structure and morphology of organic donor-acceptor photovoltaic cells based on DIP and C_{60} — •Monika Rawolle[1], David Magerl[1], Jan Perlich[2], Stephan V. Roth[2], Andreas Opitz[3], Mark Gruber[3], Julia Wagner[3], Wolfgang Brütting[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany — [2]HASYLAB at DESY, 22603 Hamburg, Germany — [3]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

A promising candidate for energy conversion utilizing organic semiconductors in small-molecule photovoltaic cells is diindenoperylene (DIP) as a new donor material in combination with the fullerene C_{60} as an electron acceptor [1].

In this contribution we investigate the influence of substrate temperature on the domain size of thermally evaporated DIP and C_{60} molecules in planar as well as in bulk heterojunctions. With Grazing-Incidence Small-Angle X-ray Scattering (GISAXS) information on horizontal and vertical structures are obtained. The real space structure information is measured with atomic force microscopy and compared with the reciprocal space investigations. Higher substrate temperatures allow growing of DIP films with higher crystallinity and increasing lateral structure sizes up to several 100 nm which serves as template for crystalline growth of C_{60} in planar heterojunctions. Even in co-evaporated films large lateral structure sizes are observed giving a large scale phase separation.

[1] J. Wagner et al. Adv. Func. Mater. (2010), early view.

CPP 8.20 Mon 17:30 P2

Structural investigations of liquid crystalline Perylene-diester benzimidazole — •Gaurav Gupta[1], Mathis Muth[2], Peter Kohn[1], Thomas Thurn Albrecht[1], and Mukundan Thelakkat[2] — [1]Institute für Physik Martin Luther Universität Halle — [2]Applied Functional Polymer University of Bayreuth

Discotic liquid crystals typically comprise a rigid aromatic core and flexible peripheral chains where the structure of the core determines the optical and intramolecular electronic properties, while the flexible side chains are decisive for self assembly and processibility from solution. As part of a side chain polymer the electro-optical properties of the discotic can be combined with the mechanical, film forming properties of a polymer. We here present the structural and optical characterization of a new liquid crystal model compound Perylene-di-ester benzimidazole(PDBI) and its polymer (PPDBI) based on XRD, DSC ,UV/Vis spectroscopy. In comparison to a common Perylene Bisimide and its side chain polymer, PDBI shows an extended absorption spectrum and a less ordered, columnar liquid crystalline phase.

CPP 8.21 Mon 17:30 P2

XRD investigation of organic disordered oligothiophene films — •Chris Elschner, Alexandr Levin, Christian Koerner, Moritz Riede, and Karl Leo — IAPP, TU Dresden

Organic small molecule semiconducting devices are well suited for optoelectronic applications like OLED (organic light emitting diode) or OSC (organic solar cell). Here, we focus on the arrangement of the molecules in the organic thin film layers, especially in the case of structurally disordered films like mixed layers. Single layers tend to show a higher degree of crystallinity in comparison to mixed layers which are often amorphous. The tool for our investigations is X-ray diffraction in grazing angle geometry combined with the pair distribution function analysis, which gives information about the short-range order of amorphous matter as well as the long-range order in the case of crystalline matter. In detail, we investigate in C60 and oligothiophene single-layers and correlate these results with a 1:1 mixed layer of these materials. As result we obtain information on the loss of crystallinity and show micro-structural information about the arrangement of the molecules in the disordered layer.

CPP 8.22 Mon 17:30 P2

The role of molecular design for optimized morphology in or-

ganic solar cells — •Christoph Schuenemann, Joerg Alex, Jan Meiss, Wolfgang Tress, Karl Leo, and Moritz Riede — IAPP, TU Dresden

Diindenoperylene (DIP) is a well known organic semiconductor which is also an attractive absorber material for applications in small molecule organic solar cells. We have synthesized Ph4-DIP, a new derivative, consisting of the DIP core and four phenyl rings attached to the two indeno-groups. To compare these two similar molecules, DIP and Ph4-DIP, we characterize the morphology of thermally evaporated thin films using x-ray diffraction and atomic force microscopy. Pristine films and mixed layers with C60 (1:1 by volume) relevant for bulk heterojunction solar cells are deposited at different substrate temperatures. Whereas DIP forms highly crystalline pristine and DIP:C60 blend layers, Ph4-DIP is found to grow amorphous even at substrate temperatures of 110°C in pristine and Ph4-DIP:C60 blend layers. These results highlight the strong influence of the molecular design on the molecular arrangement in organic thin films. The stacking of the Ph4-DIP molecules is disturbed by the four phenyl rings that are tilted with respect to the flat DIP core. The DIP molecules without these phenyl rings, however, are able to stack very densely and form large crystallites. These morphological differences can explain the diverse performance of organic solar cells made from DIP and Ph4-DIP due to different exciton diffusion length and charge carrier mobilities.

CPP 8.23 Mon 17:30 P2

Influence of substrate heating on excited state generation rates and lifetime in organic solar cells studied by photoinduced absorption spectroscopy — •Hannah Ziehlke[1], Christian Koerner[1], Roland Fitzner[2], Egon Reinold[2], Peter Bäuerle[2], Karl Leo[1], and Moritz Riede[1] — [1]IAPP, TU Dresden — [2]Institut für Organische Chemie II und Neue Materialien, Uni Ulm

The performance of organic solar cells crucially depends on the separation of photogenerated excitons into free charge carriers. The dissociation process is sensitively influenced by the nanomorphology of donor (D) and acceptor (A) phases in the photoactive blend layer. Closed percolation paths have to be present such that the created charges are able to leave the blend layer, but also the crystallinity of the D- and the A-phase influence exciton dissociation on a molecular scale. Substrate heating during the vacuum deposition of the active layer is a method to influence the thin film morphology that can lead to improved device performance. We here characterize dicyanovinyl capped quinquethiophenes (D) deposited on substrates at different temperatures (30 and 80° C). Photoinduced absorption spectroscopy (PIA) is used to determine excited state lifetimes and generation rates.We find that efficient charge separation occurs in blends with C_{60} (A) and identify the observed excited states as donor cations and triplet excitons. Heating the substrate results in an increased lifetime of the donor cation on the one hand and a decrease in the generation rate of cations on the other hand. The PIA results are complemented by solar cell devices as well as morphological studies.

CPP 8.24 Mon 17:30 P2

Influence of the exciton generation profile within the active layer on organic solar cell performance — •Wolfgang Tress, Mauro Furno, André Merten, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, TU Dresden, Dresden, Germany

As the device thickness of an organic solar cell (50...200 nm) is below the coherence length of sunlight, interference effects play an important role. An optimization of the solar cell stack is commonly done with respect to high photocurrents. Here, we go one step further and analyse not only the integral effect of sun light absorption, but additionally the effect of the spatial absorption profile within a 50 nm thick ZnPc:C_{60} bulk heterojunction device. The absorption profile is manipulated by applying transparent spacer layers with varied thicknesses. We observe a significant change of fill factor (FF) and a slight change of the open circuit voltage (V_{oc}), depending on the position of the absorption maximum in the layer. Simulation data of optical (transfer-matrix) and electrical (drift-diffusion) modelling explain this behaviour, which is mainly caused by an imbalance in charge carrier mobilities, that is determined by the blend composition. The effect can be enhanced by using spectrally narrow illumination via monochromatic LEDs to obtain a sharper generation profile in the active layer. Hence, the spatial absorption profile also explains the dependence of FF and V_{oc} on illumination colour in these devices. As consequence, the spectral mismatch factor, which is very important when properly characterizing an organic solar cell under simulated sunlight, depends on the applied voltage.

CPP 8.25 Mon 17:30 P2

External and internal quantum efficiency determination of small molecule organic tandem solar cells — •Ronny Timmreck, André Merten, David Wynands, Jan Meiss, Wolfgang Tress, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, TU Dresden, 01062 Dresden, Germany

Measuring external quantum efficiency (EQE) is an important method for characterizing solar cells. In addition to its relevance for the spectral mismatch correction of solar cells, it yields deep insight into different physical processes in solar cells because many different measurement parameters can be varied independently. Hence, especially for organic solar cells it is an important technique to get a better understanding of the underlying physics.

We perform systematic studies of the EQE of single and tandem heterojunction organic solar cells by varying the wavelength and intensity of the bias illumination. Furthermore, the bias voltage that is applied to the solar cell during measurement is varied such that for every working point of the solar cell IV-characteristics an EQE spectrum can be obtained. Both requires the use of lock-in techniques for detecting the current response of the solar cell to the chopped monochromatic light on top of the bias illumination.

Our results show a strong influence of the bias voltage on the EQE-spectrum implying that optimization of organic solar cells should be done considering EQE at maximum power point and not short-circuit. With our measurements, it is furthermore possible to independently determine the IV-characteristics of the subcells of a tandem solar cell.

CPP 8.26 Mon 17:30 P2

Water and oxygen induced degradation of small molecule organic solar cells — •Martin Hermenau[1], Kion Norrman[2], Frederik Krebs[2], Karl Leo[1], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik, TU Dresden, George-Bähr-Str. 1, 01069 Dresden, Deutschland — [2]Risø National Laboratory for Sustainable Energy, Technical University of Denmark, Roskilde, Denmark

Small molecule organic solar cells are studied with respect to water and oxygen induced degradation by mapping the spatial distribution of reaction products to elucidate the degradation patterns and failure mechanisms.

Time-of-flight secondary ion mass spectrometry (TOF-SIMS) and X-ray photoelectron spectroscopy (XPS) in conjunction with isotopic labeling using $H_2{}^{18}O$ and $^{18}O_2$ provides information on where and to what extent the atmosphere has reacted with the device. A comparison is made between the use of a humid (oxygen free) atmosphere, a dry oxygen atmosphere, and a dry (oxygen free) nitrogen atmosphere during testing of devices that are kept in the dark and devices that are subjected to illumination. It is found that water significantly causes the device to degrade. The two most significant degradation mechanisms are diffusion of water through the aluminum electrode resulting in massive formation of aluminum oxide at the Al/BPhen interface, and diffusion of water into the ZnPc:C_{60} layer where ZnPc becomes oxidized. Finally, electrode diffusion is found to have no or a negligible effect on the device lifetime.

CPP 8.27 Mon 17:30 P2

Study of trap charge in bulk heterojunction organic solar cell structures using impedance spectroscopy — •Debdutta Ray, Lorenzo Burtone, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany

In this study we use impedance spectroscopy to directly observe and estimate the trap charge density in an operating organic solar cell. Since the carrier collection efficiency in an organic solar cell is directly proportional to the electric field present in the device, the electric field may undergo distortion in the presence of space/trap charge thereby affecting the short circuit current and the fill factor. Space charge formed by photogenerated carriers has been observed, albeit indirectly, from photocurrent-voltage (IV) characteristics until now. However, when using IV characteristics, the interpretation depends on the model used. Capacitance, on the other hand, is a direct measure of the spatial distribution of the electric field inside the device. In this work we measure the capacitance as a function of voltage and frequency in solar cells under illumination. The frequency dependence provides information regarding the energetic distribution of the trap charge. The voltage dependence yields estimation of the trap charge concentration. From experiments, we estimate the lower limit of the trap charge concentration to be approximately 6x10^16 cm^-3 in ZnPc/C60 bulk heterojunction solar cells. The photocurrent-voltage characteristics of the devices can be explained with the capacitance response and the data complements each other.

CPP 8.28 Mon 17:30 P2

Diindenoperylene derivatives as green donors for organic solar cells — •Felix Holzmueller, Joerg Alex, Jan Meiss, Christoph Schuenemann, Wolfgang Tress, Markus Hummert, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, Technische Universität Dresden, 01069 Dresden, Germany

Clean energy production is one of the most challenging problems of this century. Organic solar cells (OSC) may contribute to a sustainable solution, providing a cost-efficient way to convert sunlight into electrical power. For high OSC performance, a full coverage of a broad part of the solar spectrum is necessary, which will require materials with blue, green, and red absorption.

Here, we present a series of diindenoperylene derivatives (DIPD) as green donors for OSC. We study the structure-property relationship by investigating their molecular properties and morphology of thin films, and then incorporating such materials into OSC.

Both type and size of DIPD sidegroups are found to significantly influence molecular stacking and absorption properties. We relate these results to OSC with C60 as acceptor with high open circuit voltages of around 1V and fill factors of up to 75%. The device efficiency is limited by the exciton diffusion length, which can be approximated from systematic thickness variations in flat heterojunction (FHJ) OSC. Bulk heterojunction and FHJ devices yield power conversion efficiencies of over 2% and are promising for application in tandem OSC with additional materials covering the red spectrum.

CPP 8.29 Mon 17:30 P2

Fluorinated hexaazatrinaphthylene (HATNA) derivatives as electron transport materials for organic solar cells — •Franz Selzer[1], Christiane Falkenberg[1], Martin Baumgarten[2], Manuel Hamburger[2], Klaus Müllen[2], Karl Leo[1], and Moritz Riede[1] — [1]TU Dresden, Institut für Angewandte Photophysik, George-Bähr-Str. 1, 01062 Dresden, Germany — [2]Max Planck Institute for Polymer Research, 55128 Mainz, Germany

For optimizing small molecule organic solar cells the so-called p-i-n concept is a versatile approach. Here, the photoactive donor-acceptor heterojunction is sandwiched between a transparent p-doped hole transport layer and an n-doped electron transport layer. The transport layers not only facilitate the charge carrier extraction but also act as window layers shifting the maximum of the optical interference pattern to the absorbing layers. While there are a number of well suited hole transport materials, the choice of transparent electron transport materials (ETM) with high electron mobility and conductivity as well as thermal and morphological stability is very limited. Here, we present fluorinated hexaazatrinaphthylene (HATNA) derivatives as ETM in p-i-n type solar cells in comparison with the commonly used n-doped C60 or chlorinated HATNA. While C60 absorbs in the visible range of the sun spectrum, HATNA has an optical band gap of 2.9eV. Doping with either acridine orange base (AOB) or NDN1 (Novaled AG) leads to an increase of the conductivity by several orders of magnitude to $\sigma > 1 \cdot 10^{-6}$ S/cm. Finally, we show that it is possible to replace n-C_{60} in the solar cell stack by n-doped fluorinated HATNA.

CPP 8.30 Mon 17:30 P2

Infrared absorbing materials for organic solar cells — •Matthias Holzschuh[1], Toni Müller[1,3], Roland Gresser[1], Jan Meiss[1], Günter Schnurpfeil[2], Dieter Wöhrle[2], Markus Hummert[1], Karl Leo[1], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, 01069 Dresden, Germany — [2]Institute of Organic and Macromolecular Chemistry, University of Bremen, 28334 Bremen, Germany — [3]now at Heliatek GmbH, Treidlerstrasse 3, 01139 Dresden, Germany

A contribution to the future power supply in the days of global warming and enhanced CO_2 emission might be the organic solar cells (OSC) as they provide a cost-efficient way to convert sunlight into electrical power. One way to improve OSC performance is to extend the absorption from the visible region of the solar spectrum (which can be harvested with current materials) into the infrared, a spectral region which is hardly used at the moment.

We incorporate a series of modified tin-phthalocyanines and different benz-annulated aza-bodipys as donor molecules into vacuum deposited SM-OSC, showing a thin film absorption above 700nm. We test different device configurations with C_{60} as acceptor. To gain understanding of the structure-property relationships, we additionally investigate molecular donor layers using AFM and SEM, and we study the influence of substrate heating during evaporation. Despite low open circuit voltages of about 0.4 V, we believe that the materials may be good candidates for tandem devices with complementary absorption to enhance efficiency.

CPP 8.31 Mon 17:30 P2

Influence of the molecular structure of electron transport materials on the performance of organic solar cells — •Christiane Falkenberg, Markus Hummert, Selina Olthof, Christoph Schuenemann, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, TU Dresden, 01069 Dresden

The synthesis of new functional molecules is an important approach for improving the performance of organic electronic devices. Here, understanding the link between the molecular structure and the physical properties of the materials plays a key role. We present a series of small molecules with a naphthalenetetracarboxylic diimide core and different side groups. All materials are designed to be applicable as transparent electron transport materials (ETM) in p-i-n type organic solar cells. In particular, we investigate the influence of the side chain length on basic physical properties like absorption, energy level position, morphology, and the enhancement of lateral conductivity of vacuum deposited thin films by molecular n-type doping. The latter shows the largest variations ranging from $< 10^{-8}$ S/cm (hexyl) to 10^{-4} S/cm (no side chains). Finally, we compare the performance of the synthesized materials as ETM in organic solar cells. Depending on the side chain length power conversion efficiencies of 0.01% to 2.1% are reached.

CPP 8.32 Mon 17:30 P2

Tetrapropyl-tetraphenyl-diindenoperylene derivative as new donor for organic solar cells — •Jan Meiss, Martin Hermenau, Wolfgang Tress, Markus Hummert, Christoph Schuenemann, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany

We show a diindenoperylene derivative (P4-Ph4-DIP) as green donor for heterojunction organic solar cells (OSC). OSC are characterized by current voltage, EQE, and ageing measurements. Devices with C_{60} as acceptor display very high fill factors FF of over 76% and open circuit voltages V_{OC} of 0.99 V. A clear influence of donor thickness td on short circuit current density J_{SC} and FF is visible: with $t_d = 9$ nm, J_{SC} is enhanced from 1.8 mA/cm^2 (reference device with only C_{60} as absorber) to 2.6 mA/cm^2, reaching FF = 75.7% with $V_{OC} = 0.98$ V ($\eta = 1.9 \pm 0.1$%). At higher t_d of up to 63 nm, photocurrent and FF decrease, ultimately dropping below the characteristics of the reference device. We find an EQE of 23% at the position of the donor main absorption peaks (493 nm, 525 nm, and 568 nm), reaching highest efficiencies at t_d of 9 - 12 nm and then decreasing with higher t_d. We attribute this to a limited exciton diffusion length L_D in the donor: at high t_d, the material absorbs photons, but excitons do not reach the heterointerface for dissociation and thus cannot contribute to the photocurrent. By combining measured J(V) data with calculations, we show that $L_D = (9 \pm 1)$ nm fits well to the experimental findings. Ageing experiments show that the resulting devices are highly stable when exposed to accelerated ageing.

CPP 8.33 Mon 17:30 P2

Nanowire Networks as a Transparent Electrode for Organic Solar Cells — •Christoph Sachse, Yong-Hyun Kim, Lars Müller-Meskamp, and Karl Leo — Institut für Angewandte Photophysik, Dresdner Innovationszentrum Energieeffizienz, TU Dresden, 01062 Dresden, Germany

For a broad application of organic thin film solar cells, inexpensive roll-to-roll processing on flexible and lightweight substrates is desirable. On these flexible substrates, commonly used ITO electrodes do not show satisfying performance due to the brittle nature of anorganic oxides.

Among other alternatives, recently some promising results using silver-nanowires as a conductive layer were published [1]. Such close-meshed metal grids are capable of combining the high conductivity of metals with the transparency caused by low surface coverage. Ontop, the solution based process guarantees low manufacturing costs.

Here, we evaluate and improve this alternative electrode material for organic solar cells. We achieve suitable film homogeneities with a simple dip or spray-coating process on different substrates. After post-processing an ITO-like performance is obtained.

Apart from the optimization of the electrode parameters, the thin organic solar cell stack imposes special requirements on the electrode technology. Therefore, our established small molecule technology [3] is used to evaporate organic solar cells on the nanowire electrodes and measure their performance to find suitable combinations.

[1] J.-Y. Lee, et al., Nano Lett. 8, 689 (2008).

[2] M. Riede, et al., Nanotechnology 19, 424001 (2008).

CPP 8.34 Mon 17:30 P2

Alternative Electrode Concepts and Materials for Organic Solar Cells

— •Lars Müller-Meskamp[1], Christoph Sachse[1], Yong Hyun Kim[1], Michael Machala[1], Olaf Hild[2], Christian May[2], and Karl Leo[1,2] — [1]Institut für Angewandte Photophysik, Dresdner Innovationszentrum Energieeffizienz, Technische Universität Dresden, George Bähr Straße 1, 01069 Dresden, Germany — [2]Fraunhofer Institut für Photonische Mikrosysteme, Maria-Reiche Strasse 2 01109 Dresden, Germany

Organic photovoltaics, reaching efficiencies around 8% (Heliatek, Solarmer), have become a promising technology for future energy supply. It has the potential to be cost-effective, to use little material and to utilize advanced thin film production methods like roll to roll manufacturing. Requirements for producing such a low-cost and flexible product include a highly transparent, flexible electrode. Looking for alternatives to the dominant oxide electrodes, transparent, conductive electrodes were prepared by PEDOT:PSS deposited from solution, by deposition of metal nanowires, and by a combination thereof. As recently demonstrated by us, solvent treated PEDOT electrodes can be successfully integrated into OPV cells, showing similar performance than ITO. The application of conductive metal nanoparticles, e.g. silver nanowires as random mesh electrode is showing even better performance. Low sheet resistances and good transmission can be achieved in a percolation network of high aspect ratio nanowires with low space-fill ratios.

CPP 8.35 Mon 17:30 P2

Photolithography in the service of organic electronics

— •Alex Zakhidov, Hans Kleemann, Björn Lüssem, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, Germany

Organic electronic materials have attracted interest due to their facile processing that creates tantalizing prospects for new fabrication techniques such as ink-jet printing to deliver materials only where needed. Photolithography, the gold standard process of the microelectronics industry, has received relatively little attention for the patterning of organics. The recent commercialization of organic light emitting diodes (OLEDs) in flat panel displays, however, involved their integration with silicon circuitry. Similar heterogeneous integration is envisioned in other emerging applications such as large area electronics. The ability to use photolithography to pattern all layers will enable simpler fabrication using already existing infrastructure, as well as the realization of device architectures currently not achievable using separate patterning techniques for organic and inorganic layers.

References:

1. Al.A. Zakhidov et al., Adv. Mat. 20, 3481 (2008)
2. J.-K. Lee et al., J. Am. Chem. Soc., 130, 11564 (2008).
3. Y.-F. Lim et al., J. Mater Chem. 19, 5394 (2009).
4. P.G. Taylor et al., Adv. Mat. 21, 2314 (2009).

CPP 8.36 Mon 17:30 P2

White top-emitting OLEDs using organic colour-conversion layers for improved colour-stability

— •Tobias Schwab, Simone Hofmann, Michael Thomschke, Björn Lüssem, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01069 Dresden

In contrast to white organic light-emitting diodes (OLEDs) using several vertical stacked emitters [1], the principle of down-conversion gives the chance to achieve white light with a simplified layer structure and enhanced colour stability by preventing a colour shift over lifetime due to differential aging of dyes. We investigate an approach where the conversion material is integrated into a top-emitting OLED structure in a way, that only electrons can pass this layer. This assures optical excitation and avoids unwanted electrical recombination inside the conversion layer. The emission spectra, CIE-coordinates, efficiencies, and IV-characteristics depending on the conversion layer thickness have been determined and were compared to the non-emitting host-material with similar optical properties. Lifetime measurements show that these OLEDs have almost no colour change over an investigated period up to 2200 hours. It is shown that the external quantum efficiency of the OLED does not necessarily decrease with an increased conversion layer thickness, even if the photoluminescence quantum yield of these materials is below unity. This indicates that the efficiency is improved by out-coupling of isotropic re-emitted wave-guided modes.

[1] Reineke, S et al.: White organic light-emitting diodes with fluorescent tube efficiency, *Nature*, 2009, **459**: 234-238

CPP 8.37 Mon 17:30 P2

Determination of molecular dipole orientation in organic films

— •Christian Mayr, Jörg Frischeisen, and Wolfgang Brütting — University of Augsburg, Institute of Physics, Germany

Organic light-emitting diodes (OLEDs) have been investigated for 20 years standing now at the frontier to mass production. Current research focuses on the enhancement of light outcoupling efficiency which is reduced especially by the excitation of surface plasmons (SPs) at the interface to the cathode. The orientation of molecules in films used in OLEDs has a huge effect on the coupling to SPs. Numerical simulations show that a horizontal molecular orientation with respect to the substrate can enhance the efficiency by up to 50%.

An expeditious method to determine the orientation of the transition dipole moment of molecules has been developed using angular dependent photoluminescence spectroscopy. By comparing measurement with simulations, the orientation can be quantitatively determined. Although other methods to measure molecular orientation exist, the presented method makes it not only possible to study molecular orientation in neat thin films but also of small amounts of emitters doped into a matrix material without knowing any information of the optical properties of the dopant. Hence, this method is particularly useful for the investigation of newly developed materials. Measurements of the phosphorescent emitter $Ir(ppy)_3$ doped into a CBP-matrix and of other neat and doped organic materials have been performed. With this method a deeper understanding of OLEDs and possibilities to enhance light outcoupling can be gained.

CPP 8.38 Mon 17:30 P2

A High Gain and High Charge Carrier Mobility Indenofluorene-Phenanthrene Copolymer for Light Amplification and Organic Lasing

— •Hun Kim[1], Niels Schulte[2], Gang Zhou[1], Klaus Müllen[1], and Frédéric Laquai[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Merck KGaA - Dept. OLED PC/CP, Frankfurt am Main, Germany

The combination of excellent luminescence properties, high chromophore density and partially high charge carrier mobility makes conjugated polymers suitable candidates for optically and electrically pumped light amplifiers and organic lasers. In this contribution we introduce a novel class of copolymers based on the poly(indenofluorene) backbone and investigate their photophysical as well as optoelectronic device properties. In particular, we used time-resolved optical spectroscopy to study their excited state energies and lifetimes as well as amplified spontaneous emission (ASE) characteristics in slab waveguide structures. Charge carrier mobilities were investigated by the time of flight (TOF) technique. All materials were additionally tested in organic light emitting diodes to characterize their electroluminescence efficiencies. We demonstrate that copolymers based on the poly(indenofluorene) backbone can achieve previously unprecedented gain values of about 155 cm^{-1} in combination with very high hole mobilities of up to 10^{-2} cm^2/Vs and very high electroluminescence efficiencies. This makes them ideal materials for organic lasing.

[1] H. Kim, N. Schulte, G. Zhou, K. Müllen, F. Laquai, Adv. Mater., 2010, accepted

CPP 8.39 Mon 17:30 P2

Deep Insight into the Spectroscopic Properties of a High Mobility n-type conjugated Polymer with Implications on Morphology and Charge Transport

— •Robert Steyrleuthner[1], Marcel Schubert[1], Zhihua Chen[2], Antonio Facchetti[2], and Dieter Neher[1] — [1]Universität Potsdam, Germany — [2]Polyera Corporation, USA

Electrical properties of conjugated polymers are severely influenced by the morphology of the semiconducting layer. Recently, Facchetti and coworkers reported a novel n-type polymer (Polyera ActivInk N2200) with an exceptionally high electron field-effect-mobility of up to 0.85 cm2/Vs. We could already show that the bulk mobility in this material is indeed high, though electron injection is contact limited for all used low work function cathodes. While it was initially believed that layers from N2200 are amorphous, X-ray studies by Rivnay et al. on N2200 showed an exceptional in-plane order with distinct "pi-stacking" of the naphthalene diimide cores. The purpose of our work was to study the morphology of N2200 layers prepared from different solvents and annealed at different temperatures. Information on the chain packing and layer structure was obtained by performing UV-Vis absorbance, photoluminescence, AFM and SNOM measurements on thin films and solutions. We could identify distinct absorbing species and assign them to intrachain charge-transfer excitons in the amorphous phase and to interchain excitations on aggregated chains. On this basis, conclusions regarding the morphology of the semicrystalline films are drawn and related to bulk charge transport properties.

CPP 8.40 Mon 17:30 P2

Excitonic coupling in poly(3-hexylthiophene)s - molecular weight and polydispersity effects. — Christina Scharsich[1], Anna Köhler[1], •René Kalbitz[2], Dieter Neher[2], Ruth Lohwasser[3], Mukundan Thelakkat[3], Michael Forster[4], Sybille Allard[4], and Ullrich Scherf[4] — [1]Universität Bayreuth, Experimentalphysik II, 95447 Bayreuth, Germany — [2]Universität Potsdam, Physik weicher Materie, 14476 Potsdam-Golm, Germany — [3]Universität Bayreuth, Makromolekulare Chemie I, 95447 Bayreuth, Germany — [4]Universität Wuppertal, Makromolekulare Chemie, 42119 Wuppertal, Germany

The photophysical and electronic properties of regioregular poly(3-hexylthiophene) (P3HT) are of great interest for many applications in the field of organic semiconducting materials such as solar cells and field-effect transistors. Recent research has shown that the charge carrier mobility in P3HT depends not only on the molecular weight, but also on the conformation of the polymer backbone. This was attributed to differences in the intermolecular coupling that exists in weakly aggregated P3HT chains.

By means of absorption and photoluminescence measurements in solution in combination with a Franck-Condon analysis, we determine quantitatively how the coupling strength between the chains and the fraction of aggregated chains formed depend on molecular weight, polydispersity and solvent quality. We use these data to determine the chain conformation in solution. For thin films, we show that we can control the resulting film morphology by pre-aggregates formed in solution.

CPP 8.41 Mon 17:30 P2

Temperature and Molecular Weight Dependent Structures In Poly(3-hexyl thiophene) — •Jens Balko[1], Peter Kohn[1], Ruth Lohwasser[2], Michael Sommer[2], Mukundan Thelakkat[2], and Thomas Thurn-Albrecht[1] — [1]Institute of Physics, Martin-Luther-University Halle-Wittenberg, 06120 Halle, Germany — [2]Applied Functional Polymers, Macromolecular Chemistry I, University of Bayreuth, 95440 Bayreuth, Germany

Poly(3-hexyl thiophene) (P3HT) is a common polymer semiconductor, often used as material or component in organic field effect transistors or solar cells. Despite of the extensive amount of work done on this material there are a number of important open questions concerning the structure and morphology. We performed temperature dependent scattering experiments on bulk samples of P3HT in order to elucidate the phase transitions taking place. We used chemically well-defined samples, i.e. with a very narrow distribution of molecular weights and a high degree of regiorregularity.

The measurements showed that all samples with molecular weights ranging from 5 to 34 kDa (GPC) exhibit a liquid-crystalline phase prior to melting during heating. The phase transitions also appear during cooling from the isotropic melt. While for lower molecular weight crystallization leads to the formation of extended chain crystals, around a molecular weight of 20 kDa chain folded crystals form, with the number of folds depending on the cooling rate. Moreover the close analysis of WAXS patterns allows us to estimate the degree of crystallinity.

CPP 8.42 Mon 17:30 P2

In-situ GIXRD studies of current induced structural changes of P3HT thin films — •Linda Grodd, Anton Davydok, Souren Grigorian, and Ullrich Pietsch — Solid State Physics, University of Siegen, Siegen, Germany

Conjugated polymers are of great interest for electronic applications. Especially, the poly(3-hexylthiophene) (P3HT) is a promising candidate for application in organic thin film transistors (OFETs). The correlation of electric and structural properties is essential for understanding the processes that are taking place inside the polymer, and in particular, charge transfer processes.

In-situ studies of P3HT OFETs were done by using synchrotron radiation in GIXRD geometry. The 100 reflection of a drop casted P3HT film was monitored while applying voltages between 0V and 100V to source and drain of the sample with top contacts geometry. A channel length of 2 mm ensured that the whole conducting area of polymer was illuminated by the synchrotron beam. Simultaneously to the structural studies, the current at the fixed voltage was also recorded.

The current-voltage characteristics were featuring a sudden increase of the current by several orders of magnitudes from uA range to mA range. For the latter one, a reversible change of the d(100) spacing of about 1.3% has been observed.

CPP 8.43 Mon 17:30 P2

Temperature dependent relaxation processes in MDMO-PPV films — •Henry Alberto Mendez Pinzon[1], Clara Patricia Hernandez Moreno[2], and Juan Carlos Salcedo Reyes[1] — [1]Thin Films Group, Pontificia Universidad Javeriana, Bogotá (Kolumbien) — [2]Electronics Engineering Department, Pontificia Universidad Javeriana, Bogotá (Kolumbien)

Thin films of the electroluminescent polymer MDMO-PPV were deposited on glass by means of the Doctor Blade technique. The behavior of radiative relaxation processes in MDMO-PPV films were characterized by a combination of photoluminescence and transmittance measurements in a wide range of temperatures (13K to 400K). From both types of optical measurements an unusual increase of the optical bandgap was observed. A further analysis of the spectra allows deducing structural changes in the organic film, involving segmentation of the polymeric chains, and giving rise to an improvement in the ordering of the electroluminescent layer as temperature increases. In this way, monochromatic emission from the polymer is favored after annealing.

CPP 8.44 Mon 17:30 P2

Correlation between sheet resistance and NIR-VIS absorption of PEDOT:PSS — •Felix Herrmann, Sebastian Engmann, Sviatoslav Shokhovets, Harald Hoppe, and Gerhard Gobsch — TU-Ilmenau, Ilmenau, Germany

PEDOT:PSS is a widely used buffer and hole-collecting layer in organic photovoltaics. In the past years a constant improvement of the PEDOT:PSS conductivity has been shown. This make PEDOT:PSS a potential candidate to replace ITO electrodes. Although this material is widely used in optoelectronic devices like solar cells and light emitting diodes, only little is known about the optical properties. Especially the absorption in the NIR and VIS region contains some information about free carriers and trap states in the gap. Therefore a relation between the absorption of PEDOT:PSS and the conductivity can be expected. Typically the absorption coefficient in this region is below 10^4 per cm and the film thickness reaches about 40 nm. For these small absorptions the sensitivity of standard measurement methods like transmission/reflection and ellipsometry is rather poor. Therefore ellipsometric measurements were complemented by photothermal deflection spectroscopy. The charge carrier density calculations on the basis of the absorption and dielectric function were compared with the experimentally determined sheet resistance of different films to prove that relation.

CPP 8.45 Mon 17:30 P2

Impedance spectroscopic investigations of molecularly doped conjugated polymers — •Patrick Pingel and Dieter Neher — Soft Matter Physics, University of Potsdam, Germany

Molecularly doped semiconducting polymers can exhibit exceptionally high electrical conductivity, making them suitable for use in solution-processed organic circuitry. Recently, doping of conjugated polymers with the strong molecular acceptor tetrafluorotetracyanoquinodimethane, F_4TCNQ, has been introduced [1]. It has been proposed that F_4TCNQ-doping leads to the formation of charge transfer complexes with hybrid supramolecular orbitals and a reduced band gap, and that free holes are generated via thermally-induced dissociation of these complexes. Here, thin layers of poly(2-methoxy-5-(2'-ethylhexyloxy)-*p*-phenylene vinylene), MEH-PPV, have been doped at various doping ratios. Investigation of these samples with impedance spectroscopy in a metal-insulator-semiconductor (MIS) geometry allowed us to determine both charge carrier density and mobility of the doped polymer layers. The free carrier density is found to be well below the dopant concentration, which is in full agreement to our model that free carrier formation proceeds via a charge transfer complex. Moreover, we observed the formation of an inversion layer upon depletion bias, which is absent in non-doped samples.

[1] E.F. Aziz et al., *Adv. Funct. Mater.* **2007**, 19, 3257.

CPP 8.46 Mon 17:30 P2

Near Infrared Spectroscopic Studies of Boundary Effects on n-doped Organic Semiconductor Layers — •André Merten, Moritz Riede, and Karl Leo — IAPP/TU-Dresden, George-Bähr-Straße 1,01069 Dresden

Doping of organic semiconductors is a useful method to achieve well selected charge carrier transport properties and alignment of electronic energy levels. The efficacious p-i-n concept for small molecule organic light emitting diodes or solar cells is based on the doping of the electron- and the hole-transport layers in which the active layer is embedded. Besides providing appropriate conductivity, the doping reduces injection or extraction barriers between the organic layers or organic layers and the contacts, respectively, by adjusting energetic levels. Highly doped organic layers are also used as very efficient conversion contact in organic tandem solar cells.In this study we focus on the near infrared absorption properties of n-doped organic layers on ITO or in organic layers stack like solar cells. We found a considerable elevated near infrared absorptance if the n-doped organic materials were evaporated directly on ITO, which is in contradiction to the optical constants of the ITO and of the doped materials which were determined on glass substrate. This effect will allow an inside on the elevated charge carrier concentration and the shape of the energetic bands on the organic layer-ITO boundary. As example for the consequence of this effect on small molecule organic solar cells, the IV and spectral response characteristics of device in the inverted p-i-n design, using n-C60 as ETL is discussed.

CPP 8.47 Mon 17:30 P2

Investigating the effect of molecular doping on the energy levels using Seebeck measurements — •Torben Menke[1], Peng Wei[2], Zhenan Bao[2], Karl Leo[1], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik (IAPP), TU Dresden, 01062 Dresden, Germany — [2]Stanford University, CA 94305, USA

Molecular doping plays an essential role in small molecule based organic devices like solar cells or light-emitting diodes, because it allows to control the Fermi level in the doped layers with the corresponding advantages. However the exact mechanisms of molecular doping are still far from being fully understood.

We investigate the influence of doping in different material combinations of dopants and host materials. Seebeck measurements are used to study the energetic distance between Fermi energy and transport level of doped charge transport materials, e.g. fullerene C60 or N,N,N',N'-Tetrakis(4-methoxyphenyl)-benzidine (MeO-TPD). For n-doping of C60 a novel airstable dopant is presented.

For MeO-TPD and C60 a shift of the energetic distances from 180 meV down to 30 meV and from 120 meV down to 25 meV, respectively, is observed when increasing the doping concentration. Furthermore the influence of the temperature on conductivity and Seebeck measurements is shown. For MeO-TPD and C60 the activation energies of the conductivity are found to shift from 310 meV down to 210 meV and from 240 meV down to 60 meV, respectively, with increased doping concentration.

CPP 8.48 Mon 17:30 P2

HTL based SAM-system with improved carrier injection — •Merve Anderson, Sylvia Gang, Benjamin Friebe, Björn Lüssem, and Karl Leo — IAPP, TU Dresden

Organic electronics have received an increasing interest due to their mechanical flexibility, versatile chemical design and possibility of low-cost production. Various organic devices like light-emitting diodes (OLEDs), photovoltaics (OPVs), field-effect transistors (OFETs), and memory are already on the way to commercial applications.

The performance and lifetime of these devices are dependent on both the properties of the materials as well as the interfaces between the organic layers and between organic and inorganic layers (Ma et al.,Adv. Funct. Mater., 2010, 20, 1371-1388). In particular the control of the characteristic of the metal/organic injection contact is essential for reaching a high performance in these devices.

To optimize the injection contact, we synthesised a novel class of molecules that are based on a commercial hole transport material (HTL) and are able to assemble from solution onto metal electrodes. We characterized Au-electrodes modified with these self-assembled monolayers (SAMs) by UPS/XPS, and studied the perfomance of bottom electrode OFETs with pentacene as the active layer.

With this new SAM we achieve an enhanced OFET performance in terms of a low contact resistance, increased mobility and on/off ratio compared to conventional SAMs such as Perfluorodecanethiol (PFDT) (Boudinet et al., Organic Electronics, 2010, 11, 227-237) and Pentafluorobenzenethiol (PFBT).

CPP 8.49 Mon 17:30 P2

Real time growth studies of organic-inorganic semiconductor hybrid structures — •Christopher Weber, Sebastian Bommel, and Stefan Kowarik — Institut für Physik der Humboldt Universität, 12489 Berlin, Deutschland

We combine time resolved optical and x-ray in situ methods to investigate the growth of organic semiconductor thin films on inorganic semiconductor substrates. We use organic molecular beam deposition (OMBD) to grow the organic semiconductor diindenoperylene (DIP) on three different ZnO surfaces. X-ray methods like X-Ray Reflectivity (XRR) and Gracing Incidence X-Ray Diffraction (GIXD) allow to determine the molecular alignment and roughness of the thin films. We also investigate the growth dynamics by simultaneous real time monitoring of anti-Bragg growth oscillations on different points in reciprocal space (q-space). Meanwhile optical methods like Differential Reflectance Spectroscopy (DRS) and Fluorescence Spectroscopy allow us to investigate the interdependency between structural and spectral changes during thin film growth. In this way we are able to study the correlation between molecular alignment and different surface termination of the substrates.

CPP 8.50 Mon 17:30 P2

Soft x-ray linear dichroism to explore molecular orientation in STXM — •Stephan Wenzel[1], Andreas Späth[1], Benjamin Watts[2], and Rainer H. Fink[1] — [1]ICMM, Dept. Chemie & Pharmazie, Univ. Erlangen, Egerlandstraße 3, D-91058 Erlangen, Germany — [2]Paul Scherrer Institut, Swiss Light Source, CH-5232 Villigen, Switzerland

Soft x-ray near-edge x-ray absorption fine structure (NEXAFS) is an ideal fingerprint tool for the study of organic substances. This also serves as an excellent contrast mechanism for scanning transmission x-ray microscopy (STXM). Linear dichroism which originates from the anisotropy of NEXAFS resonances further serves as a tool for the study of molecular orientation. We present some microspectroscopic studies of TCNQ and F4-TCNQ, which are commonly used in organic electronic devices. Single crystals were prepared from saturated solutions on commercial ultrathin Si3N4 membranes and imaged in the PolLux STXM at the Swiss Light Source (SLS). We discuss analytical routines to derive the molecular crystal packing in individual nano- and microcrystals from hyperspectral images, e.g., from a series of images recorded at various photon energies (corresponding to a measurement of the NEXAFS spectrum in each pixel of the image series). Such studies can be extended to more complex materials like e.g. oriented polymers in organic solar cells, where the combination of structural and chemical analysis is inevitable. The PolLux STXM is supported by the BMBF (contract 05 KS7WE1).

CPP 8.51 Mon 17:30 P2

Photoionization cross section weighted DFT simulations as promising tool for the investigation of the electronic structure of open shell metal-phthalocyanines — •Michael Vogel, Felix Schmitt, Jens Sauther, Bennedikt Baumann, Anna Altenhof, Stefan Lach, and Christiane Ziegler — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schroedinger-Strasse 56, D-67663 Kaiserslautern Tel.: +49-631-205-2855 Fax: +49-631-205-2854 E-mail: cz@physik.uni-kl.de

The valence band structure of different metal-phthalocyanines (MePcs) was investigated by comparing ultraviolet photoelectron spectra (UPS) at different excitation energies with simulated spectra that take the different photoionization cross sections at these energies into account. The Kohn-Sham eigenvalue spectra, derived from density functional theory (DFT) calculations, using hybrid exchange-correlation functionals, were weighted with the photoionization coefficients in accordance with the used excitation energy. By applying these techniques the differences in the photoelectron spectra using He I and He II radiation can be reproduced and investigated. It will be shown that the 3d-orbitals of the used metal central atom of these molecules have a major influence. The changes at different excitation energies were studied for Fe, Co, and Cu central atoms to describe the chemical tailoring effects. Further the DFT calculations were used to get a detailed image of the electronic ground state.

CPP 8.52 Mon 17:30 P2

Characterization of the electronic and optical properties of 2-Aminopyrimidine-silver based crystals — •Arthur Riefer[1], Eva Rauls[1], Wolf Gero Schmidt[1], Ion Stoll[2], Jens Eberhard[2], and Jochen Mattay[2] — [1]Theoretische Physik, Universität Paderborn, 33095 Paderborn, Germany — [2]Organische Chemie I, Universität Bielefeld, 33615 Bielefeld, Germany

The importance of organic semiconductors for many applications is due to their low fabrication effort and the possibility of tuning desired functions by chemical modification of their building blocks. In general, the properties of organic materials not only depend on their organic building blocks but also on the solid state assembly of the latter. Recently, the synthesis of a new family of organic semiconductors based on pentafluorophenyl 2-aminopyrimidine and silver salts (AgX with X=$CO_2CF_3^-$, $SO_3CF_3^-$, NO_3^-) has been reported. Depending on the involved silver salt, X-Ray analysis show the compounds to be made of 1-dimensional polymer strands with different geometries and crystal groups leading to differences in the electronic and optical properties. Therefore, we have studied pentafluorophenyl 2-aminopyrimidine and the compounds with Density Functional Theory (DFT). In detail, we calculated the band structures, the (joint) densities of states, and the dielectric functions in random phase approximation (RPA). For pentafluorophenyl 2-aminopyrimidine we obtained the energies of the HOMO and LUMO, as well as the Stokes shift by means of occupation constrained DFT. The influence of many-body effects is discussed.

CPP 8.53 Mon 17:30 P2

Vibrational analysis of ethyne-linked ZnTPP dimer — •Stephan Peter Kate[1], Simona Pop[1], Norbert Esser[1], Karsten Hinrichs[1], Mathias O Senge[2], Aoife Ryan[2], Jörg Rappich[3], and Xin Zhang[3] — [1]Leibniz Institut für Analytische Wissenschaften - ISAS - e.V., Albert-Einstein-Str.9, D-12489 Berlin, Germany — [2]School of Chemistry, SFI Tetrapyrrole Laboratory, Trinity College Dublin, Dublin 2, Ireland — [3]Helmholtz-Zentrum Berlin for Materials and Energy GmbH, Institute for Silicon Photovoltaics, Kekuléstrasse 5, Berlin, 12489, Germany

Recently, porphyrin oligomers have attracted much attention as pi-conjugated organic chromophores. Their possible advantages due to their extraordinary optical and electronic properties range from biosensors and organic solar cells to organic field-effect transistors. As a result of the pi-conjugation, the low-lying HOMO-LUMO electronic transitions allows the porphyrin oligomers to collect an extended low-energy part of the solar spectrum towards NIR spectral range. This study employs micro-Raman spectroscopy for the analysis of the vibrational modes of the ethyne-linked ZnTPP (tetraphenylporphyrin) dimer in comparison to its monomer. Their resonance Raman spectra were excited with the 633 nm (1.95 eV; HeNe laser) and 458 nm (2,71 eV; Y laser) emission lines which are located in the Q- and B-band regions of the optical absorption spectrum, respectively. The presence of the Raman-active ethyne stretching mode at 2150 wavenumbers is a finger print of the ethyne bridge used in the pi-conjugation of ZnTPP dimer.

CPP 9: Poster: Biopolymers and Biomaterials

Time: Monday 17:30–19:30 Location: P2

CPP 9.1 Mon 17:30 P2

AFM Micromechanics on Spheres and Capsules from Engineered Spider Silk — •Martin Peter Neubauer[1], Claudia Blüm[2], Thomas Scheibel[2], and Andreas Fery[1] — [1]Department of Physical Chemistry II, University of Bayreuth, Germany — [2]Department of Biomaterials, University of Bayreuth

Spider dragline silk exhibits astonishing mechanical properties combining high tensile strength and elasticity. Scheibel et al. were able to biochemically synthesize and engineer the crucial proteins accounting for the characteristic features of natural spider silk. Thus, it was possible to create a variety of structures such as spheres, capsules, hydrogels, fibers and films. Future applications are seen e.g. in the field of tissue scaffolds, biocompatible coatings or drug delivery [1].

Our aim is to perform force spectroscopy experiments in order to come to a profound understanding of the mechanical properties of these new materials. As main device we are using the atomic force microscope (AFM). The colloidal probe setup allows for single sphere/capsule measurements providing us with valuable and precise information about the response of the investigated systems to a defined mechanical stress. In addition to parameters like sample stiffness or adhesion it is also possible to monitor the release behaviour of capsules as a function of the applied force. Therefore, the classic AFM is combined with a fluorescence microscope [2].

[1] J.G. Hardy, L.M. Römer, T.R. Scheibel, Polymer, 49, 4309, (2008)

[2] P.A.L. Fernandes, M. Delcea, A.G. Skirtach, H. Möhwald, A. Fery, Soft Matter, 6, 1879, (2010)

CPP 9.2 Mon 17:30 P2

Surface characterization of cellulose films and pulp by atomic force microscopy — •Christian Ganser[1,3], Oliver Miskovic[1,3], Franz Schmied[1,3], Robert Schennach[2,3], and Christian Teichert[1,3] — [1]Institute of Physics, University of Leoben, Franz Josef Straße 18, 8700 Leoben, Austria — [2]Institute of Solid State Physics, Graz University of Technology, Petersgasse 16/2, 8010 Graz, Austria — [3]CD-Laboratory for Surface Chemical and Physical Fundamentals of Paper Strength, Graz University of Technology, Petersgasse 16/2, 8010 Graz

To obtain a deeper insight into the binding mechanisms of pulp fibers in a fiber network, an atomic force microscopy (AFM) investigation was performed on cellulose films and single pulp fibers. A chemical modification of cellulose films via spincoating of hemicellulose was performed to modify the binding strength. A comprehensive roughness characterization after spincoating revealed the morphological influence.

Further, the morphology under wet and ambient conditions was investigated to follow the drying process of the pulp fibers during the production cycle on a paper machine. Here, the swelling and dewetting of single pulp fibers is studied to simulate such a cycle and to monitor morphological changes.

Supported by **Mondi** and the **Christian Doppler Research Society**, Vienna, Austria.

CPP 9.3 Mon 17:30 P2

The Salvinia effect: Measuring the water adhesion on structures of biological air retaining surfaces — •Daniel Gandyra[1], Matthias Mail[1], Aaron Weis[1], Anke Kaltenmaier[1], Matthias Barczewski[1], Stefan Walheim[1], Kerstin Koch[4], Martin Brede[3], Alfred Leder[3], Holger Bohn[2], Wilhelm Barthlott[2], and Thomas Schimmel[1] — [1]Institute of Applied Physics, Institute of Nanotechnology, and Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology — [2]Nees-Institut for Biodiversity of Plants, University of Bonn — [3]Lehrstuhl Strömungsmechanik, Fakultät für Maschinenbau und Schiffstechnik, University of Rostock — [4]Biologie und Nanobiologie, Hochschule Rhein-Waal

A novel mechanism for long-term air retention under water is found in the sophisticated surface design of the water fern Salvinia. Its floating leaves are evenly covered with complex hydrophobic hairs retaining a layer of air when submerged under water. Surprisingly the terminal cells of the hairs are hydrophilic. These hydrophilic patches stabilize the air layer by pinning the air*water interface [1]. This *Salvinia Effect* provides an innovative concept to develop biomimetic surfaces with long-term air-retention capabilities for under water applications. In order to understand this stabilization effect one has to measure the water adhesion of those structures. We show a novel method to determine the water adhesion on those surfaces.

[1] Barthlott, W.; Schimmel, T. et al.: The Salvinia paradox: superhydrophobic surfaces with hydrophilic pins for air-retention under water. Advanced Materials 22, 2325-2328, 2010.

CPP 9.4 Mon 17:30 P2

Wrinkling of cross-linked semiflexible polymer networks — •Pascal Müller and Jan Kierfeld — Physics Department, TU Dortmund, Dortmund

Filamentous protein networks and their elastic properties play an important role in cell mechanics. We simulate regular and random two-dimensional networks of crosslinked semiflexible rods in order to gain a basic understanding of wrinkling, which occurs when such networks of semiflexible polymers are sheared. Although the initial configurations are strictly two-dimensional, displacement into the third dimension results in lower energies compared to flat networks and leads to the formation of wrinkles under shear.

We find that amplitude and wavelength of wrinkles are determined by stiffness and bending rigidity of the rods as well as global parameters like the density of the network and the applied shear stress.

CPP 9.5 Mon 17:30 P2

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

We are studying a new class of biohybrid networks made of heparin, a rod-like highly charged glycosaminoglycan, and non-charged, elastic 4-star-shaped-polyethylene glycol by using experiment, theory, and simulation. We focus on the network structure by simulations and determine the defects, the functionality of heparin, and percolation threshold of the gels. Also, we develop a mean-field type model to understand the combined effects of counterions and a good solvent on the swelling properties of the gels. It has been shown that this interplay lead to nearly constant heparin concentration in the swollen gel under physiological conditions, independent of the mole-fraction at preparation while allowing large variations of the degree of swelling and storage modulus. Furthermore, we are able to predict the degree of swelling and heparin level for different molar masses of the building blocks allowing a rational design of the hydrogels. This opens the possibility to synthesize gels which allow a constant release of heparin-binding signaling molecules while independently controlling the mechanical properties to optimize matrices with both mechanical and biomolecular cues for cell replacement-based therapies.

CPP 9.6 Mon 17:30 P2

Protein reentrant condensation induced by Fe^{3+} and Al^{3+} — •Felix Roosen-Runge[1], Benjamin Heck[1], Fajun Zhang[1], Maximilian W. Skoda[2], Robert Jacobs[3], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen — [2]ISIS, Rutherford Appleton Laboratory, United Kingdom — [3]Department of Chemistry, University of Oxford, United Kingdom

Several globular proteins has been found to show reentrant phase behavior upon adding the trivalent salt Y^{3+}, i.e. they aggregate for intermediate salt concentrations but occur in stable solution both at high and low salt concentrations [1]. Here we report on results for the physiological salts Al^{3+} and Fe^{3+} for the model protein *bovine serum albumin* (BSA). From zeta potential measurements we observe a charge inversion driven by binding of salt ions on the protein surface, which clearly goes beyond the effect due to pH-change of the solution. Small-angle X-ray scattering (SAXS) provides further information on protein shape and interactions. We observe conformational changes for BSA at different salt conditions. While at low salt concentrations electrostatic repulsion dominates the interaction, this interaction is lost in the aggregation regime. For high salt concentrations charge stabilization is recovered. The findings imply a universality of the phenomenon of reentrant condensation in protein systems, pointing towards new paths of controlling the protein phase behavior.

[1] F. Zhang et al., Phys.Rev.Lett. 101, 148101 (2008); F. Zhang et al., Proteins 78, 3450 (2010)

CPP 9.7 Mon 17:30 P2

Broadscale examination of the influence of disorder on semiflexible polymers — •Sebastian Schöbl, Klaus Kroy, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig

The structure and behaviour of biological cells is essentially affected by the biomechanical properties of semiflexible polymers. In the form of networks, such as the cytoskeleton, they build up the basic scaffold of eukaryotic cells.

In order to study the mechanical properties of these highly complex systems, both interactions of the polymer with the surrounding network and further perturbing influences have to be taken into account. We investigate the equilibrium structure of semiflexible polymers in different potential landscapes by Monte Carlo simulations. The resulting properties over a wide parameter range with respect to both polymer stiffness and volume fraction of the background potential are presented. The observables taken into account are radius of gyration, end-to-end distribution, tangent-tangent-correlations and curvature distribution.

CPP 9.8 Mon 17:30 P2

Shear-flow enhanced conformational fluctuations of single-tethered DNA molecules — •Katrin Günther, Kristin Laube, and Michael Mertig — Technische Universität Dresden, Institut für Physikalische Chemie, Mess- und Sensortechnik, 01069 Dresden, Germany

Several processes in life science and nanotechnology involve the transport and manipulation of long polymers. Due to its self-recognizing and self assemling properties in conjunction with its variability in length, DNA is a useful target for verifying theoretical polymer models.

Our work focuses on analysing the thermal fluctuations of single, surface-tethered DNA molecules in hydrodynamic shear flow by fluorescence microscopy. Instead of staining DNA with conventional intercalating fluorescent dyes, known to modify DNA properties, we use quantum dots for marking and observing the free end. Conformational transformations at particular shear rates are related to the morphology model of Brochard-Wyart.

CPP 9.9 Mon 17:30 P2

Forces of Interaction between Blank, Grafted and Blank-Grafted Colloids by Using Optical Tweezers — •Tim Stangner, Christof Gutsche, Mahdy M. Elmahdy, and Friedrich Kremer — Institut für Experimentelle Physik I, 04103 Leipzig, Deutschland

Optical tweezers are experimental tools with extraordinary resolution in positioning (+/- 1 nm) a micron-sized colloid and in the measurement of forces (+/- 50 fN) acting on it - without any mechanical contact. Here, we report the direct measurements of the interactions between blank, grafted and blank-grafted colloids across three types of salts different in their valence (KCl, CaCl2, and LaCl3). The forces are repulsive at all measured distances in all three cases, decaying with distance and showed valency dependence. For the symmetric blank colloids (SiO2), the experimental data are well described by the Derjaguin-Landau-Verwey-Overbeek (DLVO) theory revealing that the effective colloidal charge decreases with increasing counterions valence. In the case of symmetric grafted colloids (SiO2 grafted with poly(acrylic acid)), the data are quantitatively described by the Jusufi et. al. model for spherical polyelectrolytes brushes which takes into account the entropic effect of the counterions. In the asymmetric case (blank against grafted) the experimental data are described by Alexander de Gennes model which only takes into account the steric force.

CPP 9.10 Mon 17:30 P2

Influence of Pulse Duration on the Polymerization Characteristic of Photosensitive Polymers and Biomolecules by Multiphoton Polymerization — •Andreas Omenzetter[1], Sascha Engelhardt[1], Martin Wehner[2], and Arnold Gillner[2] — [1]Lehrstuhl für Lasertechnik, RWTH, Steinbachstraße 15, Aachen — [2]Fraunhofer-Institut für Lasertechnik, Steinbachstraße 15, Aachen

High resolution 3D microstructures are of great interest for various applications. These structures may prove beneficial in the field of tissue engineering. Here cells, biomaterials and polymers are combined in order to replace or improve biological tissue.

We use the technique of multiphoton polymerization (MPP) which allows polymerization of a prepolymeric resin in a very confined area. For this process very high photon densities are necessary making the use of highly focused pulsed laser radiation crucial. The probability for MPP is much higher in the focal volume than in the surrounding area. That makes it possible to generate microstructures with a resolution of about 100 nm and less.

We have focused our work on the influence of laser pulse-duration on the size of the smallest possible structures, called voxels (volume pixel). For this reason we compare the influence of different laser sources with different pulse durations on voxel formation. The main advantage of longer pulses are the lower technical preconditions and thus a possibility of a turn-key machine. This will lower costs and may result in an upscaling of the otherwise slow MPP process by parallelization.

CPP 10: Poster: Charged Soft Matter

Time: Monday 17:30–19:30 Location: P2

CPP 10.1 Mon 17:30 P2

Crystallization of β-Lactoglobulin in Solution in the Presence of YCl$_3$ — •Andrea Sauter, Fajun Zhang, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Germany.

In order to understand the vitally important tasks of proteins in living organisms, knowledge of their interactions is needed. The determination of the structure of a protein by x-ray diffraction requires high quality single crystals which are not always easy to obtain. During the last years simulations, theories and experiments suggested a two-step process of protein crystal nucleation, differing from classical nucleation theory (CNT). The system we are engaged in consists of an aqueous solution of the globular protein β-Lg with YCl$_3$. A reentrant phase behavior was observed [1]: The samples show aggregation between two critical YCl$_3$ concentrations c* and c** while a uniform solution exists for concentrations below c* or above c**. Near c* crystals grow directly from solution, following CNT. Near to c** a critical temperature T$_c$ exists, above which the supernatant of a sample is clear. Below T$_c$ it becomes reversible turbid due the forming of dense liquid drops. At lower initial protein concentrations c$_p$ these are caused by critical concentration fluctuations. The formation of aggregates precedes crystal growth. At higher c$_p$ a metastable liquid-liquid phase separation occurs. Crystallization is observed afterwards in the dense phase or starting from its interface as well as in the dilute phase. This cannot be explained by CNT, instead a two-step mechanism is assumed.

[1] F. Zhang et al. Phys Rev Lett 2008, 101, 148101.

CPP 10.2 Mon 17:30 P2

Ion competition in protein solution studied with scattering techniques: SAXS, SLS and DLS — •Elena Jordan[1,2], Fajun Zhang[1], Marcus Hennig[1,2], Ralf Schweins[2], Tilo Seydel[2], Felix Roosen-Runge[1], Sara Leibfarth[1], Frank Schreiber[1], and Giovanna Fragneto[2] — [1]IAP, Universität Tübingen, Germany — [2]ILL Grenoble, France

For advances in protein science a better understanding of the protein interaction is essential. The reentrant phase behavior of proteins, induced by multivalent counterions (Y^{3+}), is a versatile example for protein-protein interactions in electrolyte solutions. At a certain YCl$_3$ concentration, c*, the proteins phase separate and at a even higher concentration, c**, the proteins redissolve with inversed surface charge [1]. We studied the effect of added NaCl on the reentrant condensation of proteins using SAXS, static and dynamic light scattering. We found that c* and c** are shifted to higher YCl$_3$ concentrations in the presence of NaCl. The decrease in the low q intensity of SAXS indicates that the attractive interaction around c* is reduced with NaCl. The monovalent ions screen the charges and stabilize the solution. Around c** the SAXS data show that the attractive interaction is enhanced upon adding NaCl. Light scattering data and simulations support the observations. We conclude, that a mixture of YCl$_3$ and NaCl can be used to fine-tune the overall interaction and phase behavior of proteins.

[1] F. Zhang, et al. Phys. Rev. Lett. 101, 148101 (2008)

[2] F.Zhang, et al. Proteins Vol. 78, 3450 (2010)

CPP 10.3 Mon 17:30 P2

Active swimming in self-generated ionic gradients — •Michael Hauber, Benedikt Sabass, and Udo Seifert — II Institut für Theoretische Physik, Universität Stuttgart, Germany

A thorough analytic understanding of phoresis in self-generated ionic gradients is still lacking. Therefore, we study here the behavior of a charged spherical particle, which emittes a charged solute with a fixed rate. The equations describing the electrical potential, the chemical potential, and the velocity field are solved through a perturbation theory for small surface charge density. The phoretic velocity of the particle is given as a closed analytical expression, obtained from the balance between electrostatic and hydrodynamic forces. It depends on the value κa, where a is the radius of the particle and κ^{-1} is the Debye screening length. The limiting results of very small values of κa (Debye-Hückel limit) and very large values (Smoluchowski limit) are derived. Further, we investigate the dependence of the particle speed on different ways of solute emission. We also take a look at the possibility of velocity reversion for varying surface charge potential.

CPP 10.4 Mon 17:30 P2

The diffusion of charged nanoparticles at the air/water interface — •Tobias Gehring and Thomas Fischer — The University of Bayreuth

The diffusion of oppositely charged nanoparticles changes differently as we change the ionic strength of the water. The diffusion is not invariant under charge reversal of the particles. We attribute this difference to the finite non vanishing surface potential of the air/water interface. The diffusion slows down with the immersion into the water. Electrodipping might be one reason for our experiment observations, however, this electrodipping force scales with the dipole-densitiy contrast of the nanoparticles and the air/water interface, not with the charge density on the particles.

CPP 10.5 Mon 17:30 P2

Dielectric Spectroscopy of Charged Soft Matter — •Pedro Armando Ojeda May, Marcello Sega, Sofia Kantorovich, Axel Arnold, and Christian Holm — Institute for Computational Physics, Pfaffenwaldring 27, 70569 Stuttgart

We present the results of MD simulations for systems of extended dipoles in presence of charged species. Static and frequency-dependent dielectric permittivities are computed employing charge structure factors, showing how it is possible to isolate the different contributions to the permittivity, namely that of dipoles, of free charges, and the cross contributions.

The results from the simulations are used to shed light on the applicability of theoretical approaches such as those of Caillol [JCP **91** 5544 (1989)] and Schroeder [JCP **126**, 084511 (2007)] for the calculation of dielectric spectra of ionic liquids.

CPP 10.6 Mon 17:30 P2

Charge transport in confined ionic liquids — •Ciprian Iacob[1], Joshua Sangoro[1], Rustem Valiullin[1], Roger Gläser[2], Jörg Kärger[1], and Friedrich Kremer[1] — [1]Institute of Experimental Physics I,University of Leipzig, Leipzig, Germany. — [2]Institute of Chemical Technology ,University of Leipzig, Leipzig, Germany.

Broadband Dielectric Spectroscopy is employed to study charge transport in ionic liquids (ILs) in silica nanoporous membranes [1-3]. The dielectric spectra are interpreted in terms of hopping of charge carriers over spatially randomly varying energy barriers. By applying the Einstein-Smoluchowski relation to the dielectric spectra, diffusion coefficients are obtained. At higher temperatures, the diffusion coefficients of the confined and bulk ionic liquids are identical for all pore sizes while ILs are observed to diffuse faster in comparison to their bulk value at lower temperatures. The results are discussed with respect to the interplay between the dynamic glass transition and charge transport in ILs.

References:

[1] C. Iacob, J.R. Sangoro, A. Serghei, S. Naumov, Y. Korth, J. Kärger, C. Friedrich and F. Kremer. J.Chem.Phys. 129, 234511 (2008).

[2] J.R. Sangoro, C. Iacob, A. Serghei, C. Friedrich and F. Kremer. Phys. Chem. Chem. Phys. 11, 913-916 (2009).

[3] C. Iacob, J.R. Sangoro, P. Papadopoulos, R. Valiullin, S. Naumov, J. Kärger and F. Kremer Phys. Chem. Chem. Phys., 12, 13798-13803 (2010).

CPP 10.7 Mon 17:30 P2

Partial oxidation of Cu(I) based ionic liquids under aerobic conditions monitored by XPS — •Angela Ulbrich[1], Marcel Himmerlich[1], Marion Stricker[2], Jörg Sundermeyer[2], and Stefan Krischok[1] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, PF 100565, 98684 Ilmenau, Germany — [2]Fachbereich Chemie, Philipps-Universität Marburg, Hans-Meerwein-Straße, 35032 Marburg, Germany

Copper (I) based ionic liquids (ILs) like $[\mathrm{Cu(Im}^n)_2][\mathrm{CuX}_2]$ (Im^n = 1-alkylimidazole; X = Cl, Br) have great potential for catalytic applications, e.g. the synthesis of dimethyl carbonate from MeOH, CO and O$_2$ [1]. The $[\mathrm{Cu(Im}^6)_2][\mathrm{CuX}_2]$ ILs are liquid at room temperature. Detailed knowledge of the electronic structure and their behaviour under environmental conditions is quite important. Due to the low vapour pressure of ILs it is possible to analyse their properties under ultra high vacuum conditions. The electronic structure of these ILs was investigated using X-ray photoelectron spectroscopy (XPS). We have handled these oxygen-sensitive ILs under inert atmosphere and besides the expected elements only traces of oxygen were detected. Generally, strong chemical modifications of [Cu(Im^6)$_2$][CuX$_2$] were identified at the near surface region after exposure to air. The oxygen amount increased strongly and two different oxidation states were observed. Also shake-up structures near the Cu 2p core level appeared in the spectra, which are indicative for Cu(II) ions. Even after long exposure to environmental conditions, copper is not completely transformed to Cu(II).

[1] M. Stricker et al., Green Chem. 2010, 12, 1589-1598.

CPP 10.8 Mon 17:30 P2

Equilibrium and non-equilibrium features in the structure of physisorbed poly(styrene sulfonate) layers — •Stephan Block and Christiane A. Helm — Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Str. 6, D-17489 Greifswald, Germany

AFM is used to measure the surface forces and to image sodium poly(styrene sulfonate) (PSS) layers physisorbed from NaCl solutions with an ionic strength ranging between 0 M and 1 M NaCl. Colloidal probe tapping mode imaging shows that domains of PSS brushes coexist with flatly adsorbed PSS. The brush area fraction increases with rising degree of polymerization. The surface forces are a superposition of steric and electrostatic forces, their respective contribution is determined by the brush area fraction.

Unexpectedly, the internal properties of the brush domains (i.e. brush thickness and average chain distance) are independent on the deposition salt concentration. They increase with rising polymer length, while the brush thickness can also be controlled by the surrounding salt concentration (equilibrium feature).

These properties suggest that flatly and brush-like physisorbed chains can be understood as two different PSS phases, whereby the ratio of both phases is controlled by the salt concentration in the deposition solution. Furthermore, the amount of brush-like physisorbed PSS chains is related to the increase in PSS surface coverage, which is also observed after addition of salt to the deposition solution with other techniques and which is extensively described in literature.

CPP 10.9 Mon 17:30 P2

Structural changes of polycation covered surfaces induced by oxygen radicals — Markus Butto, Peter Nestler, •Florian Berg, Stephan Block, and Christiane A. Helm — Inst. für Physik, Uni Greifswald, Felix-Hausdorff-Str. 6, D-17487 Greifswald

Positively charged, branched polyethylenimin (PEI) is adsorbed onto silicon wafers and attacked by hydroxyl radicals. Changes of the PEI layer are monitored on the mesoscopic length scale by Au nanoparticle (AuNP) adsorption, using AFM imaging and UV-vis absorption. Bulk diffusion controls the AuNP adsorption. A lower saturation coverage of the AuNP demonstrates a decreased positive surface charge of the PEI layer after the radical attack. Also, we find a reduced diffusion constant of AuNPs. This is attributed to conformational changes of the PEI layer.

To measure the surface forces of a PEI layer before and after a radical attack the AFM colloidal probe (CP) technique is used. The force curves of PEI layers adsorbed from pure water show that the repulsive electrostatic force dominates the interaction (DLVO theory) and PEI adsorbs flatly. After attacking the PEI layer with hydroxyl radicals, the first force curves show a steric force suggesting PEI branches dangling into solution, additionally a short ranged attraction is found. Furthermore, the surfaces appear laterally inhomogeneous.

CPP 10.10 Mon 17:30 P2

Odd-even and even-odd effect in polyelectrolyte multilayers observed with multiple angle ellipsometry — •Peter Nestler, Stephan Block, and Christiane A. Helm — Inst. für Physik, Uni Greifswald, Felix-Hausdorff-Str. 6, D-17487 Greifswald

Within a liquid cell the growth of polyelectrolyte multilayers (PEMs) by sequential adsorption of oppositely charged polyelectrolytes is observed using ellipsometry. The polyanion is poly(styrenesulfonate) (PSS), the polycation poly(allylamine hydrochloride) (PAH), and the substrate a Si wafer. The salt content is varied between 1 and 4 mol/L NaCl, the preparation temperature between 20 and 55°C. On rise of the temperature, the thickness of a polycation/polyanion bilayer increases. After each adsorption step the PEM thickness and index of refraction is determined at several angles of incidence. A film which is always immersed in aqueous solution is at least 40% thicker than a film which is dried in air. The increase in PEM thickness after an adsorption step shows an alternating pattern (even-odd effect) due to an unequal PSS- and PAH-contribution to the thickness of one double layer. At temperatures up to 45°C, the outermost PSS layer is thicker. Then a cross-over from even-odd to odd-even effect occurs, and a top PAH layer is thicker than a top PSS layer. A similar even-odd effect is observed in the refractive index of the PEM and allows an estimation of the refractive index of the outermost monolayer. At high temperature, the thicker outermost polyelectrolyte layer always has a higher water content, irrespective of its chemical nature.

CPP 10.11 Mon 17:30 P2

The 2-dimensional Lamellar Phase of PSS Adsorbed onto an Oppositely Charged Lipid Monolayer — •Thomas Ortmann, Heiko Ahrens, Jens-Uwe Günther, Frank Lawrenz, and Christiane A. Helm — Inst. für Physik, Uni Greifswald, Felix-Hausdorff-Str. 6, D-17487 Greifswald

Monolayers of cationic lipids with adsorbed polystyrene sulfonate (PSS) are studied by isotherms, grazing incidence X-ray diffraction and X-ray reflectivity. Dioctadecyldimethylammonium bromide (DODA) is used as lipid, the PSS molecular weight is varied. For a PSS concentration of 0.01 mM (with respect to the monomer concentration) in pure water Bragg peaks of flatly adsorbed, aligned PSS chains are observed for PSS both beneath the lipids in the solid (chain separation 2-2.7 nm) and in the fluid phase (chain separation 3-6 nm), the latter only if the PSS contour length Lc exceeds 10 nm. The peak position is independent of the chain length. However the isotherms depend strongly on PSS chain length: the surface pressure of the liquid/condensed phase transition is largest for the shortest PSS used (Lc = 5.5 nm) and decreases the longer the polymer gets until a limiting value is reached (contour length Lc exceeds 25 nm). The latent heat of the phase transition shows nonmonotic behaviour with an extremum at Lc = 8 nm, and levels off at Lc = 25 nm. We suggest an explanation based on the rotational entropy of very short chains, and the confinement of very long chains. First experiments with salt in the subphase show the two-dimensional lamellar phase for low molecular weight PSS and suggest a dependence of the electron density profile on the PSS contour length.

CPP 11: Poster: New Instruments and Methods

Time: Monday 17:30–19:30 Location: P2

CPP 11.1 Mon 17:30 P2

Acoustical Characterization of PVDF-Transducers for Experiments on Musical Instruments — •Marcel Kappel, Gunnar Gidion, and Reimund Gerhard — University of Potsdam, Institute of Physics and Astronomy

Polyvinylidene fluoride (PVDF) has long been known for its flexibility in applications, which is based on its robustness and variable sensor geometry. Since the acoustical impedance is similar to that of materials like plastic and wood, it can be used for non-invasive investigations of vibrating systems for instance in musical instruments. Measurements of the piezoelectric coefficient of the PVDF-sensor were carried out with respect to important parameters such as static pressure, amplitude of the dynamical force, and long term stability. In addition, we determined the frequency response of the piezoelectric polymer as sensor and actuator. Thus, we are capable of using these transducers on two different musical instruments and compare the results with the airborne sound recorded simultaneously by a condensor microphone. These measurements can hold as a showcase for the application of PVDF-sensors in vibrating systems and material science in general.

CPP 11.2 Mon 17:30 P2

Calibration and application of novel thermal cantilever in the field of polymer science — •Thomas Fischinger and Sabine Hild — Department of Polymer Science, Johannes Kepler University Linz, Altenbergerstrasse 69, 4040 Linz, Austria

To satisfy the demands of designing polymers for advanced applications more detailed information about physical and chemical properties on the microscopic scale are required. Scanning probe microscopy has shown to be an proper tool. The development of a new generation of heatable cantilevers enhances prospects also into the nano-thermal characterization. A central point in the work with such probes is an appropriate and accurate temperature calibration of the probe. In this research the influences of sample preparation and experimental set-up on the calibration have been investigated. To minimized external influences the standard method is compared to the independent calibration of tip temperature using the Raman peak location method. With our basic experimental set-up, conventional Local Thermal Analysis in an unprecedented range of scale is available, which allows the detection of transition points such as melting point and softening point, possible. However, the determination of the glass transition point has reached its limits here, and is therefore being replaced by a new technique. Dual AC Resonance Tracking is a combination of atomic force acoustic microscopy and band excitation, which enables the unambiguous detection of temperature-induced changes in the contact stiffness of the tip-surface junction.

CPP 11.3 Mon 17:30 P2

Capability of specular reflection-absorption IR spectroscopy for qualitative and quantitative analysis of organic films on metal substrates — •Georg Mayr[1,2], Sabine Hild[2], and Michaela Schatzl[1] — [1]voestalpine Stahl GmbH Linz, voestalpine-Straße 3, 4020 Linz, Austria — [2]Institute of Polymer Science, Altenbergerstraße 69, J.K. University, 4020 Linz, Austria

Specular IR-reflection-absorption spectroscopy is a convenient tool for analysis of thin films of weak absorbing materials applied to highly reflecting substrates, e.g. metals. It is readily applied for practical purposes such as the analysis of organic coatings on metal sheets. Reflection spectra exhibit peculiarities compared to transmission spectra, what becomes evident from the investigation of films with various thicknesses (2-20 micrometer). Total absorption is not observed due to surface reflection. Weak absorption bands could be evaluated quantitatively. At intense bands deviations from the transmission mode band shape occur. These special features of reflection spectra could be explained by the refractive index dispersion and the therewith connected change in reflectivity of the coating layer in the wavelength area of an absorption band combined with Lambert-Beer absorption within the organic film. Under consideration of the aforementioned effects the reflection technique is capable of quantitative investigations, e.g. evaluation of the amount of remaining reactive functions within thermoset coatings.

CPP 11.4 Mon 17:30 P2

Characterization of functionalized graphene — •Michael Enzelberger[1], Jan Englert[2], Viatcheslav Dremov[1], Frank Hauke[2], Andreas Hirsch[2], and Paul Müller[1] — [1]Department of Physics and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Germany — [2]Department of Chemistry and Pharmacy and Institute of Advanced Materials and Processes (ZMP), Universität Erlangen-Nürnberg, Germany

Covalent functionalization of graphene is a challenging task. A possible method for characterizing the reaction product is Raman spectroscopy. However its lateral resolution is limited to about 500nm. In this talk we present our scanning probe approach to this problem. Using Kelvin probe microscopy and AFM point contact spectroscopy under ambient conditions we analyzed local work function, adhesion and Young's modulus with a lateral resolution of 30 - 50 nm. We were able to correlate the spatially integrated averages of these results with the Raman spectroscopy data.

CPP 11.5 Mon 17:30 P2

Modeling Photothermal Detection, 3 Ways to make it Quantitative — •Markus Selmke, Marco Braun, and Frank Cichos — Universität Leipzig, Experimental Physik I, mona, Deutschland

Photothermal spectroscopy has been long used to quantitatively study the absorption of liquids and materials in numerous variants, such as photothermal beam deflection spectroscopy and thermal-lens spectroscopy. While recent developments have pushed the sensitivity of its microscopic counterpart up to the level of a single quantum dot or even a single molecule, the technique has lost its quantitative character due to the complexity of the signal creation in a microscopy volume. Thus a quantitative description is missing and even the simple signal shape in axial photothermal scans of single metal nanoparticles remains unclear. Here we present 3 different quantitative descriptions reproducing the photothermal detection phenomena and parameter-dependencies while providing a thorough understanding of the signal generation. Full ab-initio EM-field calculations as well as simple Ray-Optics and Diffraction treatments are shown to agree well among each other and establish the interpretation in terms of an intuitive thermal lens mechanism. Application to experiments enable the extraction of absorption cross-sections from the photothermal signal of single nanoparticles.

CPP 11.6 Mon 17:30 P2

Photothermal Detection: New Experimental Perspectives from a Quantitative Theory — •Marco Braun, Markus Selmke, and Frank Cichos — Molecular Nanophotonics Group, University of Leipzig, Linnéstraße 5, D - 04103 Leipzig

Photothermal microscopy has been used successfully for the detection of non-fluorescent nano-objects as gold nanoparticles, quantum dots or carbon nanotubes. Recently, the sensitivity of the method was improved to detect even single molecules only by absorption of light. The technique nevertheless suffers from a lack of a fundamental quantitative description. Within our group, a new Mie-like ab-initio EM-scattering theory was developed, capable to predict the photothermal signal in a quantitative manner. Experimental data will be presented supporting this theory and showing that the technique is based on the formation of a thermal nano-lens. This allows to investigate the temperature fields induced by a single optically heated nanoparticle. The gained insight opens up the opportunity of new applications of photothermal detection beyond the imaging of absorbing nano-objects. The absorption cross-section σ_{abs} may be extracted directly from the photothermal signal. Moreover, the theory suggests the application of dual focus photothermal correlation spectroscopy to probe the dynamics of absorbing nanoparticles.

CPP 11.7 Mon 17:30 P2

Imaging Polymer Nanostructures with Scanning Transmission X-ray Spectro-Microscopy — •Benjamin Watts[1], Christopher McNeill[2], and Jörg Raabe[1] — [1]Swiss Light Source, Paul Scherrer Institut, 5232 Villigen, Switzerland. — [2]Cavendish Laboratory, University of Cambridge, J J Thomson Ave, Cambridge CB3 0HE, United Kingdom.

Thin polymer films are of increasing technological importance in optoelectronic devices such as LEDs, lasers, FETs and solar cells. However, the morphology of such films is complex, often displaying three dimensional composition structure or molecular alignment effects. The structure of the polymer film incorporated into a device can strongly affect its performance characteristics, e.g. via the connectedness between of polymer domains and to the device electrodes, or due to anisotropic material properties due to molecular alignment.

Scanning transmission x-ray spectro-microscopy (STXM) has been demonstrated to be an excellent tool for the study of polymer materials due to its high spatial resolution and strong contrast based on a variety of spectroscopic mechanisms. Recent work at the PolLux STXM has demonstrated two new developments in the imaging of thin polymer films: simultaneous surface and bulk imaging via an additional channeltron TEY detector, and molecular orientation mapping via anisotropic near edge resonances.

CPP 11.8 Mon 17:30 P2

Time-resolved soft X-ray Absorption Spectroscopy of Soluted Coordination Chemistry Compounds on a Microjet — •Alexander Kothe[1], Kai F. Hodeck[1], Chris J. Milne[2], Frank van Mourik[3], Kathrin M. Lange[1], Majed Chergui[3], and Emad F. Aziz[1,4] — [1]Helmholtz Zentrum Berlin — [2]Ecole Polytechnique Federale de Lausanne — [3]Paul Scherrer Institut — [4]FU Berlin

Investigation of the spin cross-over of coordination chemistry compounds in solution permits the study of the fundamental intramolecular processes in the absence of intermolecular effects. Time-resolved soft x-ray absorption spectroscopy (XAS) gives the opportunity to investigate especially the electronic and spin structure of molecular states and their dynamics. On a sub-fs scale this was achieved by means of dark channel fluorescence yield (DCFY), where L-edge XAS on $FeCl_3$ revealed the upper limit of 1-1.5 fs for the electron transfer to the solvent. Moreover we currently establish a system of ps-laser pump and L-edge XAS as a probe at BESSY. For this experiment we use $[FeII(bpy)_3]2+$ dissolved in water. Light of 532 nm wavelength excites a metal-to-ligand-charge-transfer state, which leads to an ultrafast spin change from singlet to quintet. The latter has a lifetime of 650 ps. Using a 23 μm microjet, the setup allows to constantly renew or cycle the sample. Besides circumventing sample damage, this gives direct access to the sample in vacuum for high repetition rate fluorescence yield measurements. This experiment opens the door for investigations of the dynamics of the charge transfer in heme proteins and other biochemical systems in solutions under real conditions.

CPP 11.9 Mon 17:30 P2

Contrast enhancement in STXM micrographs based on radiation damage — •Andreas Späth[1], Jörg Raabe[2], and Rainer H. Fink[1] — [1]Friedrich-Alexander Universität Erlangen-Nürnberg, Physikalische Chemie II and ICMM, Erlangen, Germany — [2]Swiss Light Source (SLS), Paul Scherrer Institut, Villigen, Switzerland

Radiation damage is not avoidable during resonant absorption of highly-energetic intense ionizing radiation like soft x-rays. In order to quantify its effect in x-ray microspectroscopy it is crucial to evaluate material specific critical doses as upper irradiation limit to detect the chemical species of interest and not its decomposition products. In particular in soft matter specimens sample degradation is particularly important [1]. For some materials, however, radiation damage can enhance the contrast in x-ray micrographs as will be demonstrated for microtomed slices of insect eyes (xanthopan morganii predicta). We can demonstrate that radiation energy dependent contrast enhancement is observed due to selective mass loss in anatomically different regions. The studies are completed by dose dependent studies of ultrathin polymer films and polymer bilayers with specific emphasis on the resonant and non-resonant excitations. We will employ these effects to quantify the contrast enhancement in STXM micrographs. In-situ AFM studies at the NanoXAS instrument offers direct correlations with local thickness variations [2]. The work is funded by the BMBF, contract 05K10WEA.

[1] J. Wang et al. J. Electron Spectrosc. Rel. Phenom. 170, 2009, 25

[2] I. Schmid et al. J. Phys. Conf. Ser. 186, 2009, 012015

CPP 11.10 Mon 17:30 P2

Quantitative determination of network porosity and degree of pore filling for inorganic-organic hybrid structures — Gunar Kaune[1], Martin Haese-Seiller[2], Reinhard Kampmann[2], Jean-Francois Moulin[2], Qi Zhong[1], and •Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany — [2]Institut für Werkstoffforschung, Helmoltz Zentrum Geesthacht, 21502 Geesthacht, Germany

In hybrid solar cells an inorganic semiconductor such as titania is in contact with a photoactive and semiconducting polymer. To achieve a large interface between both, bicontinuous network structures are very promising. We investigate the infiltration of a titania network structure with poly(N-vinylcarbazole) (PVK). The titania films show a hierarchical pore structure with mesopores 52 nm in size and additional large macropores with a diameter of about 180 nm. With the new method time-of-flight grazing incidence small-angle neutron scattering (TOF-GISANS) the quantitative porosity and the degree of pore filling are determined for different infiltration approaches [1].

[1] Kaune et al; J. Poly. Sci. Part B. 48, 1628-1635 (2010)

CPP 11.11 Mon 17:30 P2

First microbeam GISAXS Experiments at the new MiNaXS beamline P03 at PETRA III — Adeline Buffet[1], Mottakin Abul Kashem[1], Gunthard Benecke[1,2], Ralph Doehrmann[1], Rainer Gehrke[1], Gerd Herzog[1], Volker Koerstgens[3], Jan Perlich[1], Monika Rawolle[3], Andre Rothkirch[1], Matthias Schwartzkopf[1], Kai Stassig[1], Peter Mueller-Buschbaum[3], and •Stephan V. Roth[1] — [1]Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, D-22607 Hamburg, Germany — [2]MPIKG Golm, Abt. Biomat., Wissenschaftspark Potsdam-Golm, D-14424 Potsdam, Germany — [3]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany

The new Micro- and Nanofocus small- and wide angle X-ray Scattering undulator beamline (MiNaXS) P03 at the high-brilliance third-generation synchrotron radiation source PETRA III combines in a unique way low divergence and a microfocus and additionally a nanofocus beam. Being commissioned in 2010, the microfocus end station is operational. Using a microfocus beam size of 22x12μm^2, a SAXS resolution of >100nm has already been achieved. We prove its versatility by combining in-situ the microfocus with grazing incidence SAXS (GISAXS) and imaging ellipsometry [1]. We present first results on in-situ experiments, utilizing the high time- and spatial resolution for drop-casting experiments, and give an outlook on the novel possibilities for investigating in real time structure formation upto mesoscopic length scales. [1] Koerstgens et al., Anal. Bioanal. Chem. 396, 139 (2010)

CPP 11.12 Mon 17:30 P2

The new beamline BL-1 at DELTA — •Thorsten Brenner, Daniela Lietz, Michael Paulus, Ulf Berges, Christian Sternemann, and Metin Tolan — Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund.

Deep x-ray lithography is a method to produce various microstructures with a height up to several millimeters. Structures with a lateral resolution up to 2 μm and a high aspect ratio of about 100 can be produced. A well-established process for production of microstructures using lithography is the LIGA process. A wafer covered with a photo sensitive material is exposed through a mask. This mask consists of an x-ray transparent material and an absorber material. The lateral shape of the absorber is transferred into the photoresist by shadow projection. After chemical development the exposed (pos.) or unexposed (neg. resist) material is removed. Afterwards, the micromechanical components can be produced by electroplating and molding.

In 2010 the construction of beamline BL-1 at DELTA has been finished. This beamline uses white radiation generated by a 1.5 T bending magnet (critical energy 2.2 keV). First lithography exposures of SU-8 covered silicon wafers at BL-1 were performed successfully. The exposure times have been between five and ten minutes yielding a deposited bottom dose of 15 to 25 J/cm^3 (top to bottom dose ratio $\approx$ 5). SEM images of the developed wafers show high quality structures concerning the adhesion between resist and substrate, aspect ratio, and wall roughness. Systematic studies to find optimal exposure parameters are planned for 2011.

CPP 11.13 Mon 17:30 P2

A new set-up for fast reflectivity measurements at BL9 of DELTA — •Florian Wirkert, Julia Nase, Michael Paulus, Christian Sternemann, Sebastian Tiemeyer, and Metin Tolan — Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund

We report on a new setup for fast reflectivity measurements at beamline 9 of DELTA. A PILATUS-100k detector with a sensitive area of 83.8×33.5 mm^2 and a high dynamic range allows to obtain a complete reflectivity on a single TIFF image. The main difference to classical reflectivity measurements is that the detector remains fixed at its position while the sample is tilted continuously from 0° to an angle $\theta_{\max}$. As first test measurements we investigated the adsorption of the protein lysozyme at the solid-liquid interface between a silicon wafer and water. In a sequence of reflectivities taking 55 s each, we could demonstrate the temporal evolution of protein adsorption at a solid-liquid interface. Thus this set-up provides a strong tool for the investigation of time-dependent processes by x-ray reflectivity measurements.

CPP 11.14 Mon 17:30 P2

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 wiggler 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 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. grazing incidence wide angle X-ray scattering (GIWAXS), 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 in transmission or reflection, i.e. dip-coating with GISAXS, 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 and give an outlook on upcoming activities.

CPP 11.15 Mon 17:30 P2

Molecular orientation in soft matter thin films studied by resonant soft x-ray reflectivity — •Peter Reichert[1], Markus Mezger[1], Blandine Jérôme[2], and Jeffrey B. Kortright[2] — [1]Max-Planck-Institut für Polymerforschung, Mainz — [2]Materials Sciences Division, Lawrence Berkeley National Lab., USA

Polarization resolved Resonant Soft X-Ray Reflectivity is a novel technique to study depth profiles of molecular orientation in soft matter thin films with nanometer resolution. It combines the chemical sensitivity of Near-Edge X-ray Absorption Fine Structure spectroscopy to specific molecular bonds and their orientation with respect to the polarization of the incident beam with the precise depth profiling capability of X-ray reflectivity. We show polarization dependent reflectivity data from side chain liquid crystalline polymer thin films and their quantitative analysis using the Berreman formalism. Further examples on buried films and amorphous polymers where the orientation is induced by the free surface and the substrate demonstrate the capabilities of the technique.

CPP 11.16 Mon 17:30 P2

CIDNP study of cyclic peptides with sulfur containing amino acids — •Talea Köchling[1], Gerald Hörner[1], Alexandra Yurkovskaya[2], and Hans-Martin Vieth[1] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — [2]International Tomography Center of SB RAS, 630090, Institutskaya 3a, Novosibirsk, Russia

Combining NMR spectroscopy with the effect of spin hyperpolarisation opens new ways to get information about structure of radicals and their reaction pathways. A way for creating transient non-thermal signal amplitudes is chemically induced dynamic nuclear polarisation (CIDNP) resulting from the formation of a radical pair of a photo-excited dye molecule and a quencher, e.g. an amino acid residue. The dependence of CIDNP on the external magnetic field allows to determine magnetic resonance parameters (hyperfine coupling constants and g-factor) of elusive radicals. On the other hand from its time dependence with microsecond resolution it is possible to differentiate geminate and bulk processes, so that reaction pathways and rate constants can be extracted.

In the present study, CIDNP results for different peptides containing a combination of methionine, methylcysteine and glycine in aqueous solution at ambient temperature are obtained. By comparing these peptides that differ in their sulfur-backbone-distances and number of thioether units differences in radical structure and reaction kinetics are shown and discussed. In particular, primary and secondary reaction steps are differentiated and rate constants are determined.

CPP 11.17 Mon 17:30 P2

Spin-Flip NMR Spectroscopy as a Tool for Structure Investigations — •Günter Hempel and Matthias Roos — Martin-Luther-Universität, Institut für Physik, Betty-Heimann-Straße 7, D-06120 Halle

We propose a NMR procedure which can give information about molecular structure also in disordered systems. This method is based on polarization exchange between neighboured 1H nuclei. The exchange rate is proportional to the coupling constant which depends on length and orientation of the spin-spin connection vector with respect to the magnetic field.

Because of the particular structure of the effective Hamiltonian, the oscillations survive relatively long time which can lead to rather high accuracy of the determination of the frequency and subsequently of the structural parameters. Coarsely spoken, we burn holes into the proton polarization and follow the subsequent re-filling of the holes. In microsecond range the oscillatory behaviour mentioned above is observed, and at millisecond scale spin-diffusion processes dominate.

This method was applied to liquid-crystal compounds to study certain bond angles in the mesomorphic phases which are not accessible by scattering methods. Furthermore, we could estimate spin-diffusion constants in liquid crystals and polymeric materials.

CPP 11.18 Mon 17:30 P2

NMR Signal Averaging in 62 Tesla Pulsed Fields — •Benno Meier[1], Sebastian Greiser[1], Jürgen Haase[1], Thomas Herrmannsdörfer[2], Frederik Wolff-Fabris[2], and Joachim Wosnitza[2] — [1]University of Leipzig, Faculty of Physics and Earth Science, Linnéstrasse 5, 04103 Leipzig, Germany — [2]Hochfeld-Magnetlabor Dresden, Forschungszentrum Dresden-Rossendorf, 01328 Dresden, Germany

Nuclear Magnetic Resonance (NMR) experiments at up to 62 Tesla in pulsed high magnetic fields at the Hochfeldlabor Dresden-Rossendorf are reported. The time dependence of the magnetic field is investigated by observing various free induction decays (FIDs) in the vicinity of the maximum of the pulse. By analyzing each FID's initial phase and its evolution with time the magnetic field's time dependence can be determined with high precision. Assuming a cubic dependence on time near the field maximum its confidence is found to be better than ± 0.03 ppm at low fields and ± 0.8 ppm near 62 Tesla. The obtained time dependence of the field can be used to demodulate and phase correct all FIDs so that they appear phase locked to each other. As a consequence signal averaging is possible. The increase in signal-to-noise is found to be close to that expected theoretically. This shows that the intrinsic time dependence of these pulsed field can be removed so that the NMR signals appear to be taken at rather stable static field. This opens up the possibility of performing precise shift measurements and signal averaging also of unknown, weak signals if a reference signal is measured during the same field pulse with a double-resonance probe.

CPP 11.19 Mon 17:30 P2

Universal Long-Time Behavior of Spin Echo — •Benno Meier[1], Jonas Kohlrautz[1], Boris Fine[2], and Jürgen Haase[1] — [1]University of Leipzig, Faculty of Physics and Earth Science, Linnéstrasse 5, 04103 Leipzig, Germany — [2]University of Heidelberg, Institute for Theoretical Physics, Philosophenweg 19, 69120 Heidelberg, Germany

Nuclear magnetic resonance (NMR) is a versatile tool also for the investigation of many-body dynamics in quantum mechanics. Here we report on preliminary measurements of free induction and solid echo decays of ^{19}F spins ($I = 1/2$) in an isolated cubic lattice (CaF_2). In agreement with a recently developed generic theoretical description we find that the long-time decay of both solid echo and free induction decay (FID) is described by an exponentially decaying oscillatory function where exponential decay rate and frequency of oscillations are the same for both the FID and the solid echo and do not depend on the initial state of the spin system at the end of the pulse sequence. This behaviour supports the notion of eigenvalues of time evolution operators in chaotic many-body quantum systems.

CPP 12: Organic Semiconductors II: Solar Cells B (jointly with HL, DS)

Time: Tuesday 10:30–13:00 Location: ZEU 222

Topical Talk CPP 12.1 Tue 10:30 ZEU 222

Modelling charge transport in organic semiconductors — •Denis Andrienko — MPI for Polymer Research, Mainz, Germany

The role of material morphology on charge carrier mobility in partially disordered organic semiconductors is discussed for several classes of materials: derivatives of hexabenzocoronenes,[1] perylenediimides,[2] triangularly shaped polyaromatic hydrocarbons,[3] Alq3,[4] polypyrrole and a variety of organic crystals. Simulations are performed using a package developed by Imperial College, London and MPI for Polymer Research, Mainz (www.votca.org[5]). This package combines: quantum chemical methods for the calculation of molecular electronic structures and reorganization energies; molecular dynamics and systematic coarse-graining approaches for simulation of self-assembly and relative positions and orientations of molecules on large scales; kinetic Monte Carlo and master equation for studies of charge transport.

[1]. J. Kirkpatrick, V. Marcon, J. Nelson, K. Kremer, D. Andrienko, *Phys. Rev. Lett.*, 98, 227402, 2007

[2]. V. Marcon, W. Pisula, J. Dahl, D. W. Breiby, J. Kirkpatrick, S. Patwardhan, F. Grozema, D. Andrienko, *J. Am. Chem. Soc.*, 131, 11426, 2009

[3]. X. Feng, V. Marcon, W. Pisula, M. R. Hansen, J. Kirkpatrick, F. Grozema, D. Andrienko, K. Kremer, and K. Müllen, *Nature Materials* 8, 421, 2009

[4]. A. Lukyanov, D. Andrienko, *Phys. Rev. B*, 82, 193202, 2010

[5]. V. Rühle, C. Junghans, A. Lukyanov, K. Kremer, D. Andrienko, *J. Chem. Theor. Comp.* 5, 3211, 2009

CPP 12.2 Tue 11:00 ZEU 222

Performance of density functional theory for donor-acceptor

systems: a case study for TTF and TCNQ molecules — •Viktor Atalla[1], Mina Yoon[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Oak Ridge National Laboratory, USA

Organic materials are promising candidates for a next generation of electronic devices, since they offer a variety of new intriguing properties. However, from a theoretical point of view these materials are challenging because they are often composed of donor-acceptor systems, for which density-functional theory (DFT) with state-of-the-art exchange-correlation (XC) functionals is often suspected to fail. Here we study the performance of DFT in describing electron affinities, ionization potentials, and charge transfer for clusters of the prototypical electron donor molecule TTF and acceptor molecule TCNQ.

For the indivdual molecules we calculate the dependence of the HOMO and LUMO levels on the fraction of exact exchange and the screening length [1]. We find that conventional semilocal and hybrid XC functionals severely underestimate HOMO-LUMO gaps. For weakly bound TTF-TCNQ dimers all investigated XC functionals consistently give charge transfer from the donor to the acceptor, however the amount of transfered charge is strongly functional dependent - in particular all semilocal functionals have significant aritificial charge transfer in the asymptotic limit.

[1] A. Krukau *et al.*, J. Chem. Phys. **125**, 2006

CPP 12.3 Tue 11:15 ZEU 222

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

We present external quantum efficiency (EQE) studies of P3HT:PCBM based bulk heterojunction polymer solar cells with improved intensity resolution in the sub-bandgap (SBG) region, i.e. the energy range below the optical bandgaps of the pristine materials. Varying the P3HT:PCBM blending ratio, we find that in addition to a Gaussian profile an exponential tail is needed for a quantitative description of the SBG EQE spectra. To gain insights into the origin of the single contributions, absorption and emission spectra covering several decades of intensity and SBG EQE signals are discussed in detail.

CPP 12.4 Tue 11:30 ZEU 222

Quantitative analysis of optical spectra and solar cell performance of P3HT:PCBM blends — •Sarah T. Turner, Patrick Pingel, Robert Steyrleuthner, and Dieter Neher — Institute of Physics and Astronomy, University of Potsdam, Germany

The properties of solar cells made from a blend of regioregular poly(3-hexylthiophene) (P3HT) with [6,6]-phenyl-C_{61}-butyric acid methyl ester (PCBM) are known to depend largely on the layer morphology. Here, we present the results of optical studies on P3HT:PCBM blends coated from chloroform and dichlorobenzene with subsequent thermal annealing. A recently established analytical model developed by Spano for the absorption of weakly interacting H-aggregates was used to obtain information about the fraction of crystallized chains, the width of the aggregates, and the energetic disorder in the P3HT phase [1]. In terms of an increased aggregate width and a decreased energetic disorder in the P3HT phase, thermal annealing was found to have little effect on the films prepared from dichlorobenzene and an appreciable effect on the films prepared from chloroform. The results from the model were compared with the performance of solar cell devices and single-carrier devices with the same active layer. Most importantly, the initial increase in P3HT aggregate size upon thermal annealing showed a good correlation with an increase in hole mobility. Further increases in solar cell device performance at higher annealing temperatures were correlated with a decrease in P3HT energetic disorder and an increase in PCBM aggregation.

[1] F.C. Spano, J. Chem. Phys. 2005, 122, 234701.

CPP 12.5 Tue 11:45 ZEU 222

Influence of Phase Segregation on the Dynamics of Charge Carriers in Organic Solar Cells — •Andreas Baumann[1], Tom J. Savenije[3], Dharmapura H. K. Murthy[3], Martin J. Heeney[4], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), Am Hubland, D-97074 Würzburg — [3]Optoelectronic Materials Section, Department of Chemical Engineering, Delft University of Technology, 2628 BL Delft, The Netherlands — [4]Department of Chemistry, Imperial College London, London, SW7 2AZ, United Kingdom

The morphology of a bulk heterojunction solar cell plays an important role in the dynamics of charge carriers, whereas the donor–acceptor ratio have a great impact on the extent of phase segregation. A fine phase intermixing is believed to be beneficial for an efficient photogeneration. However, the charge transport is strongly related to percolated pathways to the electrodes. We studied the influence of phase segregation on the dynamics in the blend system poly(2,5-bis(3-dodecyl thiophen-2-yl) thieno[2,3-b]thiophene) (pBTCT) mixed with [6,6]-phenyl-C61-butyric acid methyl ester. We used the technique of charge extraction by linearly increasing voltage and transient microwave conductivity to study the macroscopic and microscopic transport properties, respectively. We found an enhanced geminate recombination in the 1:1 ratio blends due to fine phase intermixing, whereas extensive phase segregation in the 1:4 ratio led to an efficient polaron pair dissociation.

CPP 12.6 Tue 12:00 ZEU 222

Charge separation at molecular donor-acceptor interfaces: correlation between interface morphology and solar cell performance — •Andreas Opitz, Julia Wagner, Mark Gruber, Ulrich Hörmann, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Combinations of organic electron and hole conductive materials are widely used for ambipolar charge carrier transport and donor/acceptor photovoltaic cells. Thereby the efficiency of these excitonic solar cells is correlated to the morphology of the interface between the donor and the acceptor materials.

In this contribution we show the effect of crystallization behaviour on molecular bulk and planar heterojunction solar cells [1]. Different donor (copper phthalocyanine – CuPc, diindenoperylene – DIP) and acceptor (Fullerene – C_{60}, per-fluorinated copper phthalocyanine – F_{16}CuPc) materials are analysed for their growth morphology in planar and mixed films as well as for their performance in photovoltaic cells. The morphology of the blended layer ranges from molecularly mixed films in the case of the two phthalocyanines to phase-separated films when mixing CuPc or DIP with C_{60}. A corrugated interface is found for bilayered structure of DIP/C_{60} [2]. Additionally a good crystallization behaviour of DIP improves the solar cell performance even for its lower absorption in comparison to CuPc.

[1] A. Opitz et al., IEEE J. Sel. Top. Quant. (2010), early view.

[2] J. Wagner et al. Adv. Func. Mater. (2010), early view.

CPP 12.7 Tue 12:15 ZEU 222

Towards Ideal Morphology of Polymer Bulk Heterojunction Solar Cells — •Chetan Raj Singh[1], Michael Sommer[2,3], Marcel Himmerlich[1], André Wicklein[3], Stefan Krischok[1], Mukundan Thelakkat[3], and Harald Hoppe[1] — [1]Institute of Physics, Ilmenau University of Technology, Germany — [2]Department of Chemistry, University of Cambridge, United Kingdom — [3]Applied Functional Polymers, University of Bayreuth, Germany

We present the thorough optimization of block copolymer (BCP) based polymer solar cells utilizing a blend of a self-assembling P3HT-b-PPerAcr BCP and an PPerAcr acceptor homopolymer. As an effect of increasing acceptor content in the block copolymer/homopolymer blend, we observe a continuous rise in the open circuit voltage (Voc) and the short circuit current (Isc) leading to an overall improved photovoltaic performance. The improved performance with increasing acceptor content is attributed to (a) an increase of the acceptor domain size leading to improved charge transport and to (b) a reduced recombination of charge carriers at the cathode interface due to the surface segregation of the acceptor. The surface segregation of the acceptor is identified by atomic force microscopy and X-ray photoelectron spectroscopy. Furthermore we show that by deliberately introducing an acceptor buffer layer at the cathode interface, we are able to control Voc at relatively high values (˜ 640 mV), independently of the bulk heterojunction morphology underneath.

CPP 12.8 Tue 12:30 ZEU 222

Triplet Excitons and Cations in dicyanovinyl end-capped quaterthiophenes with varying side chain length — •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, Technische Universität Dresden — [2]Institut für Organische Chemie II und Neue Materialien, Universität Ulm

Dicyanovinyl end-capped oligothiophenes (DCV-nT) are highly suitable for systematical investigations of energy and charge transfer processes in donor-acceptor blends because of the tunability of electronic and morphological properties by varying e.g. length of backbone or side chains. Moreover, it has been shown to work well as absorber in small molecule organic solar cells (OSC) achieving up to 5.2% power conversion efficiency (PCE) for DCV-5T in a bulk heterojunction (BHJ) device[1].

We use photoinduced absorption spectroscopy (PIA) to probe the long-living (μs-ms) excited states (triplet excitons, cations) after photoexcitation of DCV-nT:C_{60} blends. With PIA, their generation and recombination behaviour can be investigated. Here, we report our results obtained on a series of DCV-4Ts with varying side chains from none to methyl side chains which supposedly mainly influences the morphology of the thin film. We complement our studies by exploring the potential of these materials as absorber layer in planar and BHJ solar cells. For example, DCV-4T without side chains gives an open circuit voltage of 1V and PCEs of 1.9% in a BHJ solar cell with C_{60}.
[1] Fitzner et al., Adv. Func. Mat., accepted

CPP 12.9 Tue 12:45 ZEU 222

Surface structure of organic heterojunction solar cells — •M. Zerson[1], E.-C. Spitzner[1], C. Riesch[1], A. Sperlich[2], H. Kraus[2], A. Förtig[2], C. Deibel[2], V. Dyakonov[2], R. Lohwasser[3], M. Thelakkat[3], and R. Magerle[1] — [1]Chemische Physik, TU Chemnitz — [2]Experimental Physics VI, Julius-Maximilians-University of Würzburg — [3]Makromolekulare Chemie I, Univ. Bayreuth

In organic heterojunction solar cells based on P3HT and PCBM, the charge transfer within the active layer as well as the charge transport towards the electrodes are determined by the electronic properties of the interfaces and their microstructure. The surface of semicrystalline polypropylene has been shown to be covered by a thin layer of amorphous material. We aim at investigating potential similarities between organic semiconductors for photovoltaics. We report on 3D depth profiling of the surface structure of different types of P3HT and blends of P3HT with PCBM using amplitude modulation atomic force microscopy. From a map of amplitude-phase-distance 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 determined. The latter is found to be between 4 and 10 nm thick, depending on the type of material and the sample preparation conditions (thermal and solvent annealing). We discuss the impact of the thickness of the amorphous top layer on the efficiency of organic solar cells.

CPP 13: Focused Session: Confinement of Polymers in Nanoscopic Layers - How Much do Properties Change? I

Time: Tuesday 10:30–13:00 Location: ZEU 160

Invited Talk CPP 13.1 Tue 10:30 ZEU 160

Rheological Response of Ultrathin Polymer Films — •Gregory McKenna, Paul O'Connell, and Jinhua Wang — Texas Tech University, Lubbock, TX, USA

We have developed a novel bubble inflation method to determine the rheological response of ultrathin polymer films. The method shows,consistent with other methods, dramatic reductions of the glass transition (Tg) of polystyrene of high molecular weight. We have also discovered a major stiffening of the material in the rubbery plateau regime. New information for polycarbonate shows that, like polystyrene it can exhibit strong reductions in the Tg and rubbery stiffening. We also report the first evidence of terminal flow in the bubble inflation experiment using polycarbonate having thicknesses from 3 nm to 9 nm. We have also performed liquid film dewetting experiments for both polystyrene and polycarbonate systems. The results for the polystyrene are consistent with literature reports of little change in the glass transition and no change from macroscopic behavior for the rubbery plateau regime. On the other hand, for polycarbonate we observe both a reduction in the Tg and moderate stiffening in the rubbery regime. These results will be discussed in detail.

Invited Talk CPP 13.2 Tue 11:00 ZEU 160

Molecular dynamics at nanometric length-scales — •Friedrich Kremer — Universität Leipzig, Fak. f. Physik u. Geowissensch., Inst. f. Experimentelle Physik I, Linnéstr. 5, D-04103 Leipzig

Broadband Dielectric Spectroscopy, Spectroscopic vis-Ellipsometry, X-Ray Reflectometry, Alternating and Differential Scanning Calorimetry are combined to study glassy dynamics and the glass transition in nanometric thin (about 5 nm) layers of polystyrene (PS) having widely varying molecular weights and Polymethylmethacrylate (PMMA) deposited on different substrates. For the dielectric measurements two sample geometries are employed, the common technique using evaporated electrodes and a recently developed approach taking advantage of nanostructures as spacers. All applied methods deliver the concurring result that deviations from glassy dynamics and from the glass transition of the bulk never exceed margins of nearly 3 K independent of the layer thickness, the molecular weight of the polymer under study and the underlying substrate. Our findings are discussed in the context of the highly controversial literature and prove that an appropriate sample preparation is of paramount importance in order to avoid artefacts. References: 1.Erber et al., Macromolecules 43, 7729 (2010). 2.Mapesa et al., Europ. Phys. J. - Special Topics 189, 173-180 (2010). 3.Treß et al., Macromolecules (2010). DOI:10.1021/ma 102031k.

Invited Talk CPP 13.3 Tue 11:30 ZEU 160

On the origin of the deviations from bulk behavior in ultrathin polymer films: from glass transition to tracer diffusivity — •Simone Napolitano, Michael Wübbenhorst, and Cinzia Rotella — Department of Physics and Astronomy, Katholieke Universiteit Leuven, Celestijnenlaan 200D, Leuven, 3001, Belgium

We show clear evidence that the changes ultrathin films undergo during annealing are strongly correlated to the amount of chains irreversibly adsorbed at the interface. An analysis of the time evolution of the dielectric function during annealing steps above Tg revealed three different regimes: at times much shorter than the adsorption time, the thickness of the adsorbed layer is constant and the incomplete interface mimics the effect of a free surface (packing frustration); upon increase of surface coverage, the films undergo a series of metastable states characterized by the largest changes in the deviations from bulk behavior; finally the system approach a new equilibrium whose properties are fixed by the new interfacial configurations. Our picture is confirmed by further investigation of the distribution of glass transition temperatures, tracer diffusivity and dielectric relaxation strength at different distances from the adsorbing interface. We show that during annealing ultrathin films evolve towards a steady state whose properties might still differ from bulk. In particular, for polystyrene, the lack of specific interactions with the substrate results in slow adsorption kinetics, keeping the deviations from bulk behavior in steady states with an extremely long lifetime.

Invited Talk CPP 13.4 Tue 12:00 ZEU 160

Calorimetry of Thin Films – From Single Layer Glass Transitions to Inter-layer Diffusion in Double Layers — •Christoph Schick[1], Dongshan Zhou[2], and Heiko Huth[1] — [1]Institute of Physics, University of Rostock, Germany — [2]State Key Laboratory of Coordination Chemistry, Nanjing University, China

Nanocalorimetry allows studying the glass transition in nanometer thin films. One of the striking results of fast scanning (FSC) as well as alternating current (AC) calorimetry is the commonly observed constant Tg in thin films down to a few nm. Blends of polystyrene and poly(phenylene oxide) (PS/PPO) confined in thin films were investigated by AC nanocalorimetry. For this blend, we see even for the thinnest films (6 nm, corresponding to about half of PPO radius of gyration Rg) only one unchanged glass transition. The good miscibility between PS and PPO remains even in ultrathin films. Finally, we show that our chip calorimeter is sensitive enough to study the interlayer diffusion in ultrathin films. The PS chains in a 150 nm PS/PPO double layer that is prepared by spin coating PPO and PS thin films in tandem gradually diffuse into the PPO layer when heated above the Tg of PS, forming a PSxPPO(100-x) blend. However, on top of the PSxPPO(100-x) blend, there exists a stable pure PS like layer (ca. 30nm in our case) that does not diffuse into the blend beneath even staying at its liquid state over 10 hours.

CPP 13.5 Tue 12:30 ZEU 160

Chain Dynamics of Polymers Confined to Ordered Nanoporous Alumina Membranes — •Cornelius Franz[1], Salim Ok[2], Gopalakrishnan Rengarajan[2], Fabián Vaca Chávez[1], Christian G. Hübner[3], Martin Steinhart[2], and Kay Saalwächter[1] — [1]Institut für Physik - NMR, Universität Halle, Betty-Heimann-Str. 7, 06120 Halle — [2]Institut für Chemie, Universität Osnabrück — [3]Institut für Physik, Universität Lübeck

The nanoscopic confinement effect of hard neutral or attractive walls on the dynamics of polymer chains in the melt is studied by solid-state NMR. We apply a variety of NMR techniques to the characterization and the elucidation of chain dynamics in true model composites based on self-ordered nanoporous alumina with well-defined geometry and the possibility to tune the properties of the inorganic surface.

The long-time dynamics of entangled melts is significantly different from the bulk and rather anisotropic in a layer of a few nm close to the weakly interacting wall, and that the effect appears to scale with the entanglement spacing. Further preliminary studies demonstrated that these effects are orientation dependent, and also occur for nominally unentangled melts.

We also studied the large-scale diffusion by pulsed-gradient NMR and the infiltration kinetics by confocal fluorescence microscopy where we have monitored the infiltration of dye-doped polymer into self-ordered AAO in situ. Pore-wall modification experiments were verified by quantitative high-resolution NMR.

CPP 13.6 Tue 12:45 ZEU 160

Polymer melt dynamics in confinement: Reduction of the inter-chain entanglement density close to an interface — •Oliver Bäumchen, Renate Fetzer, and Karin Jacobs — Department of Experimental Physics, Saarland University, D-66041 Saarbrücken, Germany

Fluids in confinement may exhibit properties that differ strongly from bulk behavior. One example is the reduction of the glass transition temperature in thin polymer films, whether above or below the entanglement length of the polymer. Another example is the inter-chain entanglement density in the bulk compared with the one in the vicinity of an interface. Dewetting experiments of thin (<200 nm) polystyrene films reveal that the inter-chain entanglement density close to an interface can be reduced by a factor 3 to 4, depending on interfacial properties [1,2]. Parameters that control the reduction will be detailed. Our findings shed new light on the solid/liquid boundary condition of liquid flow [3], on the molecular structure of this interface and possible reasons for a reduction of the glass transition temperature.

[1] O. Bäumchen, R. Fetzer and K. Jacobs, *Phys. Rev. Lett.* **103**, 247801 (2009).

[2] O. Bäumchen and K. Jacobs, *Soft Matter* (2010), DOI: 10.1039/C0SM00078G.

[3] O. Bäumchen and K. Jacobs, *J. Phys.: Condens. Matter* **22**, 033102(21pp) (2010).

CPP 14: Elastomers and Gels

Time: Tuesday 10:30–13:00 Location: ZEU 114

Topical Talk CPP 14.1 Tue 10:30 ZEU 114

Network effects in nano-filled polymer systems — •Kay Saalwächter[1], Cornelius Franz[1], Kerstin Schäler[1], Salim Ok[2], Martin Steinhart[2], Aurelie Papon[3], Francois Lequeux[3], and Helene Montes[3] — [1]Institut für Physik - NMR, Martin-Luther-Univ. Halle-Wittenberg, Halle, Germany — [2]Institut für Chemie, Universität Osnabrück, Germany — [3]Physico-chimie des Polymères et Milieux Dispersés, ESPCI ParisTech, Paris, France

The effect of nanoscopic filler particles on the dynamics of linear and cross-linked chains above T_g is controversial. While often, an increase of the cross-link density in the particle vicinity was claimed, previous work of our group based on the use of low-field multiple-quantum (MQ) NMR has indicated that the homogeneity of the matrix is hardly ever affected by different types of filler [1]. However, in model-filled samples consisting of a dispersion of grafted silica particles, we found a (i) fraction of polymer with slower dynamics and (ii) a fraction with locally increased cross-link density, that both correlate with the silica specific surface. We further discuss related results for linear melt dynamics in nanoscopic model confinement provided by anodic aluminum oxide (AAO) membranes with channels of 20–400 nm diameter [2]. We consistently observe a fraction of chains with less isotropic dynamics on long time scales, behaving network-like. Our results are consistent with a layer thickness of a few nanometers at the non-interacting interface, where the geometric confinement modifies the chain modes.

[1] J. L. Valentín et al., *Macromolecules* **43**, 334 (2010).

[2] S. Ok et al., *Macromolecules* **43**, 4429 (2010).

CPP 14.2 Tue 11:00 ZEU 114

The distribution of segmental order in polymer networks — •Michael Lang[1] and Jens-Uwe Sommer[1,2] — [1]Leibniz Institut für Polymerforschung e.V., Hohe Straße 6, 01069 Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden

Recently we showed [1] that segmental order in entangled polymer networks is controlled by monomer fluctuations along the tube, which leads to a dependence $(N_e N)^{-1/2}$ for the average segment orientation of entangled chains of length $N > N_e$ in monodisperse networks, where N_e denotes the tube reorientation length. We extend this approach to derive the distribution of segmental order based on Gaussian chain conformations and randomly reorienting tubes for monodisperse samples. Furthermore, effects of polydispersity are discussed and we also include the effect of the most predominant network defects in our discussions.

[1] M. Lang, J.-U. Sommer, PRL 108, 177801 (2010).

CPP 14.3 Tue 11:15 ZEU 114

Switching kinetics of pMDEGA based thermo-responsive hydrogel films probed by in-situ neutron reflectivity — •Qi Zhong[1], Gunar Kaune[1], Monika Rawolle[1], Ezzeldin Metwalli[1], Achille M. Bivigou-Koumba[2], Andre Laschewsky[2], Christine M. Papadakis[1], Robert Cubitt[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany — [2]Universität Potsdam, Inst. Chemie, Karl-Liebknecht-Str. 24-25, 14476 Potsdam-Golm, Germany — [3]Institut Laue-Langevin, 6 rue Jules Horowitz, 38000 Grenoble, France

Stimuli-sensitive hydrogels exhibit interesting properties which attract increasing attention due to a large variety of applications such as drug delivery, sensors and bioseparation. A novel thermoresponsive poly(monomethoxy diethyleneglycol acrylate) (PMDEGA) exhibits a higher lower critical solution temperature (LCST) when compared to the frequently investigated thermoresponsive polymer poly(N-isopropylacrylamide) (PNIPAM). Thus PMDEGA can be an interesting alternative to PNIPAM in tropical countries. In order to create an internal ordering in thin PMDEGA hydrogel films, the homopolymer is replaced by a PMDEGA based tri-block copolymer with polystyrene as an end group, P(S-b-MDEGA-b-S). Homo- and tri-block polymer thin films, with thickness of 35.9 nm and 39.4 nm respectively, are prepared by spin coating. Neutron reflectivity is used to probe the kinetic behaviour of the thermo-responsive hydrogel films in temperature jumps above the LCST.

CPP 14.4 Tue 11:30 ZEU 114

Light-induced deformation of azobenzene elastomers: different molecular models — •Vladimir Toshchevikov[1,2], Marina Saphiannikova[1], and Gert Heinrich[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden, Germany — [2]Institute of Macromolecular Compounds, Bolshoi pr. 31, 199004 Saint-Petersburg, Russia

Light-sensitive elastomers bearing azobenzene chromophores in network strands have a fascinating potential for technical applications (microrobots, micropumps, artificial muscles, smart materials) due to their ability to change the shape under light irradiation. In the present work, we extend the theory [1] devoted to light-induced deformation of amorphous azobenzene polymers consisting of short oligomers to azobenzene elastomers. Different molecular models are used: a regular cubic network model and a general network model with random orientation of end-to-end vectors of network strands. We show that similar to amorphous azobenzene polymers, azobenzene elastomers demonstrate either expansion or contraction with respect to the polarization vector of the light depending on their chemical structure. Increase of the degree of croslinking results in the decrease of the magnitude of the photo-induced deformation at the same light intensity. The results of the theory are compared with experimental data for azobenzene elastomers.

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.

CPP 14.5 Tue 11:45 ZEU 114

Mechanical moduli of magneto-sensitive elastomers in a homogeneous magnetic field — •Dmytro Ivaneyko[1,2], Vladimir Toshchevikov[1], Marina Saphiannikova[1], and Gert Heinrich[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden, Germany — [2]Technische Universität Dresden, ECEMP, Marschner Str. 39, 01307 Dresden, Germany

Magneto-sensitive elastomers (MSEs) are a class of smart materials whose mechanical properties can be controlled by application of an external magnetic field [1]. Recently, MSEs have been used in mechanical systems and automobile applications such as stiffness tunable mounts and suspension devices. In the present work, we develop the theory of mechanical properties of MSEs which takes into account a non-linear elasticity of a polymer matrix. Different spatial configurations of magnetic particles within the matrix are considered: homogeneous, chain-like and plane-like. It is shown that interaction between the magnetic particles results in the contraction of an elastomer along the direction of uniform magnetic field. With increasing magnetic field the shear modulus for the shear deformation perpendicular to the magnetic field increases for all spatial configurations of magnetic particles. The Young modulus for the tensile deformation along the magnetic field decreases for the chain-like configurations and increases for the plane-like configurations with increasing magnetic field.

This work was supported by funds of Europe Union and the Free State of Saxony.

[1] Varga, Z.; Filipcsei, G.; Zrínyi, M., Polymer 2005, 46, 7779-7787.

CPP 14.6 Tue 12:00 ZEU 114

Magnetophoretic transport in thermoreversible ferrogels — •Tobias Lang[1], Marina Krekhova[2], Holger Schmalz[2], Reinhard Richter[1], and Ingo Rehberg[1] — [1]EP5, Universität Bayreuth — [2]MC1, Universität Bayreuth

The viscoelastic properties of thermoreversible ferrogels [1] can be tuned via the temperature, making such gels an exciting type of magnetic soft matter [2]. Preliminary studies with these materials showed a separation effect of gel and ferrofluid. So far magnetophoresis was studied by optical means, and limited to dilute magnetic fluids [3]. With our x-ray based technique [4], we are able to investigate magnetophoretic transport in any kind of magnetic fluid as well as in ferrogels.

Most recently, we were able to synthesize cobalt ferrite hydrogels [5]. These thermoreversible hydrogels have cubic and hexagonal mesophases which are tunable via the temperature. As a consequence, the magnetophoretic transport in different phases can be studied as a function of the viscoelasticity. For a further characterization of the samples, magnetometric and magneto-rheometric measurements have been carried out.

[1] G. Lattermann and M. Krekhova, Macromol. Rapid. Commun. 27. 1273 (2006) [2] C. Gollwitzer et al., Soft Matter 5, 2093 (2009) [3] A.S. Ivanov, A.F. Pshenichnikov, JMMM 322, 2575-2580 (2010) [4] R. Richter and J. Bläsing, Rev. Sci. Instrum. 72, 1729 (2001) [5] M. Krekhova et al., Langmuir (DOI: 10.1021/la1040823) (2010)

CPP 14.7 Tue 12:15 ZEU 114

Micro- to Mesoscale Simulation of Hydrogel Swelling Dynamics Based on a Phase field Model — •Daming Li, Hongliu Yang, and Heike Emmerich — Materials and Process Simulation (MPS), University of Bayreuth

Hydrogels consist of three-dimensional charged polymer networks, mobile ions, and solvent, and they are usually synthesized by chemically cross-linking charged polymers. Hydrogels can swell or shrink by the absorption or squeeze of solvent if it is under the external stimuli, e.g., temperatures, pH, ionic strength, etc. Stimuli-response hydrogels have attracted much attention for their potential in wide range of applications, e.g. drug delivery, biosensors, tissue engineering etc.

Here we contribute to a precise understanding of the mechanisms responsible for the hydrogels' swelling kinetics as well as dynamics by proposing for the first time a model approach that can resolve the inherent short range correlation effects along the hydrogel-solution interface jointly with the long range ionic transport fields. To that end we investigate the swelling dynamics of hydrogels, which is a moving boundary problem, by a phase field model, which couples the Nernest-Planck like equation for the concentration of mobile ions, Poisson equation for the electric potential, mechanical equation for the displacement and an equation for the phase field variable. Simulation reveals that under the chemical stimulation the hydrogel will swell or shrink if the concentration of mobile ions inside bath solution decreases or increases. This is in agreement with the experimental results qualitatively.

CPP 14.8 Tue 12:30 ZEU 114

Kinetics of structural changes in concentrated thermoresponsive blockcopolymer solutions — •Joseph Adelsberger[1], Ezzeldin Metwalli[1], Alexander Diethert[1], Achille Bivigou-Koumba[2], André Laschewsky[2], Isabelle Grillo[3], Peter Müller-Buschbaum[1], and Christine M. Papadakis[1] — [1]TU München, Lehrstuhl für funktionelle Materialien, Garching — [2]Universität Potsdam, Institut für Chemie — [3]Institut Laue-Langevin, Grenoble

Thermoresponsive polymers display strong changes in volume when heated above the lower critical solution temperature (LCST). Therefore they are interesting candidates for applications in ultrafiltration, in sensors or as drug delivery systems. We study 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]. In order to elucidate the structural changes, occuring after rapid heating above the LCST, we have performed time-resolved small-angle neutron scattering experiments with measurement times down to 0.1 s at D22 at ILL in Grenoble. The micellar radius shows a sudden decrease immediately after the LCST is crossed, i.e. the formerly hydrophilic shell shrinks and releases water. Moreover collapsed micelles form small fractal aggregates, which become denser and grow to big clusters.

[1] A. Jain, C. M. Papadakis et al., *Macromol. Symp.* **291-292** (2010), 221; J. Adelsberger, C. M. Papadakis et al., *Macromolecules* **43** (2010), 2490

CPP 14.9 Tue 12:45 ZEU 114

Elasticity of Core-Shell Microgel particles determined by AFM Technique depending on the Temperature — •Marcel Richter and Regine von Klitzing — Technische Universität 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 thermoresponsive behaviour and can therefore be classified as smart materials.

In special the mechanical properties these microgels are of great interest. Here, AFM is a suitable method for the determination of the Young's modulus [2]. We synthesised core-shell particles and investigate the change in stiffness according to the cross linker and comonomer amount. Due to the thermoresponsive behaviour of our particles the elasticity was determined in a temperature range for 20°C to 65 °C. These microgel particles are synthesized by emulsion polymerization without using any surfactants at temperature about 70°C [3]. The size of microgels is determined by Dynamic Light Scattering and Atomic Force Microscopy.

[1] K. Kratz, T. Hellweg, W. Eimer, Polymer (2001), 42, 6531 [2] E. K. Dimitriadis et al, Biophysical Journal, (2002), 82, 2798 [3] R. Pelton, Adv. Colloid Interface Sci. (2000), 85, 1

CPP 15: Organic Semiconductors III: Aggregation and Nanostructures (jointly with HL, DS)

Time: Tuesday 14:00–15:15 Location: ZEU 222

CPP 15.1 Tue 14:00 ZEU 222

Substituted Perylene Diimides as Electron Acceptors in Organic Solar Cells: Suppressing Aggregate Formation to Increase Device Efficiency — •Valentin Kamm, Glauco Battagliarin, Ian A. Howard, Michael Hansen, Hans W. Spiess, Alexey Mavrinskiy, Wojciech Pisula, Chen Li, Klaus Müllen, and Frédéric Laquai — Max-Planck-Institut für Polymerforschung, Mainz, Deutschland

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 drawback of strong aggregation leading to intermolecular excited state formation that results in exciton trapping. These traps can effectively limit the diffusion of excitons to the interface where charge separation occurs and thus strongly reduce the charge generation efficiency. In this contribution we study the influence of substitution of PDI molecules with side groups attached to the terminal and to the perylene core positions on the formation of aggregates. In particular transient photoluminescence and absorption spectroscopy are used to probe the impact of aggregation on the dynamics of charge generation and recombination in bulk heterojunction solar cells. Besides, AFM, x-ray and solid state NMR techniques are used to get further insight into the solid state morphology of polymer:PDI blends on different length scales. Finally, we correlate the photophysical properties of the PDI derivatives with the efficiency of bulk heterojunction organic solar cells and present unprecedented efficiencies from polymer:PDI solar cells.

CPP 15.2 Tue 14:15 ZEU 222

Near-field spectroscopic mapping of the nanoscale phase separation of low band-gap polymer:fullerene blend film — •xiao wang[1], hamed azimi[2], hans-georg mack[1], mauro morana[2], hans-joachim egelhaaf[3], alfred j. meixner[1], and dai zhang[1] — [1]Institute of Physical and Theoretical Chemistry, Auf der Morgenstelle 18, University of Tübingen, Germany — [2]Konarka Austria F&E GmbH, Linz, Austria — [3]Konarka Technologies GmbH, Nürnberg, Germany

We present the study of the influences of the additive 1,8-octanedithiol (ODT) on the nanometer scale morphology and local photophysics properties of low band-gap polymer blends, PCPDTBT and PCBM. Near-Field spectroscopic mapping provides the possibility to obtain simultaneously morphology and spectroscopic (photoluminescence and Raman) information correlated with high spatial resolution.[1] We observe the phase separations of the PCPDTBT:PCBM blend film induced by ODT by the dramatically increased PL emission from PCPDTBT that was originally largely quenched, by the fluctuations of spectral features at different locations of the sample surface, by the fibril-shaped topographic features evolve to spherical bumps. The correlations between the local photo physics properties and the morphology of the blend film with/without ODT at both the micrometer and nanometer scales were revealed by the confocal and high-resolution near-field spectroscopic mapping technique. 1.Wang, X.; Zhang, D.; Braun, K.; Egelhaaf, H. J.; Brabec, C. J.; Meixner, A. J. Adv. Funct. Mater. 2010, 20, (3), 492-499.

CPP 15.3 Tue 14:30 ZEU 222

High Crystallinity and Nature of Crystal–Crystal Phase Transformations in Regioregular Poly(3-hexylthiophene) — •Ovidiu F. Pascui[1,3], Ruth Lohwassser[2], Michael Sommer[2], Mukundan Thelakkat[2], Thomas Thurn-Albrecht[1], and Kay Saalwächter[1] — [1]Institut für Physik, Martin-Luther-Univ. Halle-Wittenberg, Halle, Germany — [2]Makromolekulare Chemie I, Universität Bayreuth, Germany — [3]Experimentelle Physik III, TU Dortmund, Germany

Molecular weight and stereoregularity affect the morphology and the crystallinity of conjugated polymers and are thus of pivotal relevance for the mobility of charge carriers in electro-optical device applications. We use ^{13}C solid-state NMR to determine the crystallinity and details on crystal–crystal phase transformations in regioregular head-to-tail poly(3-hexylthiophene) of well-defined molecular weight and demonstrate that the crystallinity was previously severely underestimated. Typical crystallinities are at least around 37% for the lowest molecular weights and as high as about 64% upon increasing MW, corresponding to a corrected maximum value for the reference melting enthalpy of $\Delta H_\mathrm{m} \approx 37$ J/g for use in DSC experiments. Using one- and two-dimensional NMR, we observe that the crystal-crystal phase transition between a 3D- and a 2D-ordered crystalline phase at around 60°C entails a structural disordering process of the alkyl side chains, while not affecting the backbones. The formation of the 3D-ordered phase is kinetically suppressed at higher molecular weights.

see: O. F. Pascui et al., *Macromolecules* **43**, 9401 (2010).

CPP 15.4 Tue 14:45 ZEU 222

Self-Assembled Ultralong Organic Semiconducting Nano/Microwires — Julia Lambrecht, •Tobat P. I. Saragi, and Josef Salbeck — Macromolecular Chemistry and Molecular Materials (mmCmm), Department of Mathematics and Science and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Strasse 40, D 34132 Kassel, Germany

We report on the simple process in fabrication of spiro-substituted perylene diimide nano/microwires (NMWs) by using self-assembly approach, namely drying under solvent atmosphere. This method results in a controllable number of NMWs on the substrate, which enables us to fabricate single NMW electronic device. Furthermore, we are able to control the growth direction of NMWs by using a structured substrate. An aspect ratio as high as ~9200 can be obtained in our experiment and the longest wire is determined to be 5.5 mm. The resistivity of the single NMW is characterized and the value is in the range of 100 Ohm m and 10000 ohm m.

CPP 15.5 Tue 15:00 ZEU 222

Plasmonic enhancement of light absorption in organic semiconductors using silver nanowire arrays — •Matthias Handloser[1], Ricky Dunbar[2], Philipp Altpeter[2], Lukas Schmidt-Mende[2], and Achim Hartschuh[1] — [1]Department Chemie and CeNS, Ludwig-Maximilians-Universität, München, Germany — [2]Department Physik and CeNS, Ludwig-Maximilians-Universität, München, Germany

Plasmonics can be used to improve light absorption in photovoltaic devices, permitting a considerable reduction in the physical thickness of absorber layers, and yielding new options for solar-cell design [1]. We investigated arrays of aligned silver nanowires embedded in different organic polymers via confocal microscopy in combination with Time Correlated Single Photon Counting (TCSPC) and Pump-Probe techniques. The wires had a length of 10 um, a height of 20 nm, and variable widths and spacings. Thin films of different organic semiconductors were then deposited onto these arrays. Plasmon modes were excited through one and two photon absorption between 500 to 900 nm and photoluminescence maps and transients of the arrays were recorded. We observed a clear correlation between photoluminescence intensity, lifetime and nanowire spacing. We analyzed our data to distinguish between absorption and radiative rate enhancement and energy transfer to the metal followed by quenching. [1] H.A.Atwater, A.Polman, Nature Materials 9, 205 (2010)

CPP 16: Focused Session: Confinement of Polymers in Nanoscopic Layers - How Much do Properties Change? II

Time: Tuesday 14:00–15:30 Location: ZEU 160

Invited Talk CPP 16.1 Tue 14:00 ZEU 160

Glass Transition Dynamics of Polymer Films — •Ophelia K. C. Tsui — Department of Physics, Boston University, Boston, MA 02215

Most polymers solidify into a glassy amorphous state, accompanied by a rapid increase in the viscosity when cooled below the glass transition temperature (Tg). There has been an ongoing debate on whether the Tg changes with decreasing polymer film thickness and the origin of the changes. We measured the viscosity of unentangled, short-chain polystyrene (Mw = 2.4 kg/mol) films on silicon at different temperatures and found that the transition temperature for the viscosity decreases with decreasing films thickness, in agreement with the changes in the Tg of the films observed by thermal expansion measurements. By applying the hydrodynamics equations to the films, we are able to explain the data fully by assuming that a highly mobile layer is present within the top 2.3 nm thick region of the films and follows an Arrhenius dynamics while the remaining of the films is bulk-like.

Invited Talk CPP 16.2 Tue 14:30 ZEU 160

Conformational properties of polymer melts in spatial confinement — Hendrik Meyer, Albert Johner, Joachim Wittmer, Julia Zabel, Jean Farago, and •Jörg Baschnagel — Institut Charles Sadron, Strasbourg, France

Over the last years several groups discussed deviations from chain ideality in homopolymer melts and dense solutions. These deviations result from the interplay between melt incompressibilty and chain connectivity; the strength of the effect depends on the dimensionality of space. After an introduction to the behavior in the bulk we focus on polymer melts confined to thin films and capillaries. We find that deviations from chain ideality are stronger in thin films than in bulk and even stronger in thin capillaries. These theoretical predictions will be illustrated by results from molecular simulations of simple (coarse-grained) polymer models.

CPP 16.3 Tue 15:00 ZEU 160

Substrate influence on the structure and properties of polyelectrolyte multilayers — •Chloe Chevigny, Maximilian Zerball, and Regine von Klitzing — Stranski Lab., TU Berlin, Institut für Chemie, Sekr. TC 9, 10623 Berlin

Polyelectrolyte Multilayers (PEM), made by the Layer-by-Layer (LbL) deposition technique, are a very versatile and interesting tool for many technical applications. Since their development 20 years ago, there has been an exponential increase of works in this topic, allowing a better comprehension of their structures and properties, but also more applied studies, resulting in many applications such as sensor coatings or drug delivery systems. However, in order to better understand the functionalities of these systems and find new applications, fundamental studies are always needed. We focus on the properties profile across the film and on the effect of the solid substrate: over which length scale the substrate affects the film properties, and from which distance does the film reach bulk properties? For this project several surfaces types are studied: Silicon and Gold (resp. negatively and positively charged), with or without a first protective layer of PolyEthyleneImine PEI. The structure, as well as the swelling and dynamical properties of the multilayers, are determined via a combination of ellipsometry, X-rays and neutron reflectivity, QCM-D and FRAP measurements. The substrate is found to have an important influence, both on internal structure (layers inter-diffusion increases linearly from top to bottom) and properties (changing the substrate changes both diffusion and swelling features) of the multilayers.

CPP 16.4 Tue 15:15 ZEU 160

Density in polymer films and at the polymer-solid interface — •Eicke Tilo Hoppe[1], Boyuan Wang[1], Martin Haese-Seiller[2], Jean-Francois Moulin[2], Max Port[3], Bernhard Menges[3], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Fachgebiet der weichen Materie, Garching, Germany — [2]GKSS-Forschungszentrum Geesthacht, Geesthacht, Germany — [3]MPI for Polymer Research, Material Science Group, Mainz, Germany

The change in physical behaviour of polymers at interfaces is of importance for the adhesion of polymer coatings to solids, e.g. in medical implants and in nanocomposites. The aim of the project is the investigation of the influence of the polymer-solid interaction on the physical properties of the polymers near the interface.

We focus on the correlation between the changes of density, viscosity and chain orientation of the polymer melt near the interface. Polybutadiene melts from toluene solutions on silicon oxide are studied as a model system. To tune the interface interactions between substrate and polymer melt, the substrate surface is modified chemically and by silanization. The density profile near the solid interface is investigated by time-of-flight neutron reflectometry (TOF-NR) at REFSANS. The films have a lower density than the bulk value expected from literature and density deviations at the interface. The optical properties of polybutadiene are investigated in the bulk using optical waveguide spectroscopy, whereas the interphase is characterized by monitoring the surface plasmon. The refractive index in the interphase close to the gold-coated glass is lower compared to the bulk.

CPP 17: Liquid Crystals

Time: Tuesday 14:00–15:15 Location: ZEU 114

Topical Talk CPP 17.1 Tue 14:00 ZEU 114

Modulated mesophases: from labyrinths to liquid ferroelectric chords. — •Alexey Eremin[1], Ulrike Kornek[1], Ralf Stannarius[1], Antal Jákli[2], and Hideo Takezoe[3] — [1]Otto-von-Guericke Universität, IEP/ANP, 39106 Magdeburg — [2]Liquid Crystal Institute, Kent State University, USA — [3]Dept. of Organic and Polymeric Materials, Tokyo Institute of Technology, Japan

Competition between incompatible ground states often leads to frustration, which is manifested by spatially modulated states. This phenomenon can be found in various physical and chemical systems such as semiconductors, lipid membranes, ferrofluids, or superconductors. Here we show an example of a polarization modulated liquid crystal phase exhibiting a variety of fascinating structures. Those include labyrinths of layer dislocations in free-standing films and stable ferroelectric fibres with liquid-like order of molecules in cylindrically wrapped layers. Using non-linear optics and polarising microscopy we get insight into the internal organisation of the polar structure of the phase in different geometries as well as the mechanical properties the fibres.

CPP 17.2 Tue 14:30 ZEU 114

Reconfigurable knots and links in chiral nematic fluids — •Uroš Tkalec[1,2], Simon Čopar[3], Miha Ravnik[3,4], Slobodan Žumer[3,2], and Igor Muševič[2,3] — [1]Max-Planck-Institute for Dynamics and Self-organization, Göttingen, Germany — [2]Jožef Stefan Institute, Ljubljana, Slovenia — [3]Faculty of Mathematics and Physics, Ljubljana, Slovenia — [4]Rudolf Peierls Centre for Theoretical Physics, Oxford, United Kingdom

Creation and control of non-trivial topological objects is important in various biological and condensed matter systems. However, detailed studies of knotted structures in all these systems remain challenging due to their inherent smallness and typically large but poorly controllable ensemble of configurations. We show that knots and links of fascinating complexity can be realized and specifically reconfigured in the molecular orientational field of chiral nematic liquid crystal using optical manipulation of topological defect loops, which are spanned on ordered microparticle arrays. We also unveil a simple reknitting mechanism, based on a tetrahedral rotation of two relevant disclination segments, that allows us to predict and topologically characterize all available entangled configurations. These principles reveal a novel manifestation of knot theory in a concrete physical phenomenon and offer a way to interpret akin topological structures in physically analogous condensed matter systems.

CPP 17.3 Tue 14:45 ZEU 114

Morphological evolution of pi-walls in nematic liquid crystals under microfluidic flow — •Anupam Sengupta, Stephan Herminghaus, and Christian Bahr — MPI-DS, Bunsenstrasse 10, 37073, Goettingen

Microflows of pure nematic liquid phase are studied by the authors using polarizing microscopy and fluouroscence confocal polarizing microscopy.Varying the combinations of surface anchoring, channel dimensions and flow rates, different textures and defect structures evolve: stable, unstable or flow-stabilized. The authors use the forces present when such systems flow through an appropriate microfluidic device to manipulate the structures. Novel colloidal systems dispersed in nematic matrices, can selectively be transported over large length scales, using the nematic bulk or the flow-induced textures and defect structures.

CPP 17.4 Tue 15:00 ZEU 114

Entropy-driven enhanced self-diffusion in confined reentrant supernematics — •Marco Mazza — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany

We present a molecular dynamics study of reentrant nematic phases using the Gay-Berne-Kihara model of a liquid crystal in nanoconfinement. At densities above those characteristic of smectic A phases, reentrant nematic phases form that are characterized by a large value of the nematic order parameter $S \simeq 1$. Along the nematic director these “supernematic” phases exhibit a remarkably high self-diffusivity which exceeds that for ordinary, lower-density nematic phases by an order of magnitude. Enhancement of self-diffusivity is attributed to a decrease of rotational configurational entropy in confinement. Recent developments in the pulsed field gradient NMR technique are shown to provide favorable conditions for an experimental confirmation of our simulations.

Ref.: M.G. Mazza, M. Greschek, R. Valiullin, J. Kaerger, M. Schoen, Phys. Rev. Lett. 105, 227802 (2010).

CPP 18: Poster: Transport and Spectroscopy in Molecular Nanostructures (Intersectional Session with MO)

Time: Tuesday 18:00–20:00 Location: P1

CPP 18.1 Tue 18:00 P1

Structure and Spectroscopy of Perylene Bisimide Aggregates — David Ambrosek, •Sergey Bokarev, and Oliver Kühn — Institut für Physik, Universität Rostock, Germany

Perylene bisimides (PBIs) are excellent dyes and versatile building blocks for supramolecular structures. Only recently have PBIs been shown to depict absorption characteristics specific to J-aggregates. In contrast to the exciton trapping observed in H-aggregates, these systems could potentially be used in transferring energy captured from the sunlight to artificial reaction centers. We apply electronic structure calculations to investigate monomeric and aggregate geometries as well as electronic properties in gas phase.

The PBI monomeric excitation spectrum has been assigned based on time-dependent Density Functional Theory (DFT) calculations for the geometry-optimized electronic ground state structure. The two lowest $\pi - \pi^*$ type transition at 582 nm and 453 nm are found to be in excellent agreement with experiment. A shoulder in the experimental spectrum around 550 nm is assigned to result from a vibrational progression involving several vibrational normal modes. The electronic coupling within a dimer is analyzed in terms of a supermolecule approach, paying attention to the influence of charge transfer states, as well as using monomeric transition densities. Dimer and hexamer structures are also discussed on the basis of the dispersion-corrected tight-binding DFT method.

CPP 18.2 Tue 18:00 P1

Transient Absoption of Pheophorbide-a Supramolecular Complexes Determined in a Mixed Quantum-Classical Description — •Jörg Megow, Yaroslav R. Zelinskyy, Beate Röder, and Volkhard May — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, D-12489 Berlin, Germany

A mixed quantum classical approach for the calculation of nonlinear optical properties of large chromophore complexes in solution is proposed. The complex is formed by a butanediamine dendrimer to which four pheophorbide-a molecules are covalently linked. While all nuclear coordinates are described classically by carrying out room-temperature MD-simulations the electronic excitations are treated quantum mechanically utilizing a Frenkel-exciton model. The computations are applied to study transient absorption measured in a pump-probe scheme. Different signatures of excitation energy redistribution appearing on a 1 to 5 ps time scale* are uncovered.

*J. Megow et al., Theodor Förster commemorative issue, ChemPhysChem (submitted)

CPP 18.3 Tue 18:00 P1

Anomalous strong exchange narrowing in excitonic systems — •Jan Roden and Alexander Eisfeld — MPI-PKS Dresden

Whenever electronic transitions interact with an environment, i.e. they are affected by static or dynamic disorder, the absorption lines are broadened. However, if several of those electronic (two-level) systems are coupled so that they exchange excitation, the absorption spectrum can be strongly narrowed compared to the absorption of the uncoupled systems. This remarkable phenomenon, the so-called exchange narrowing, has been observed already several decades ago in the absorption spectra of molecular aggregates – it is responsible for the narrow shape of the well-known J-band of organic dye aggregates (J-aggregates).

Often the number of coherently coupled monomers is estimated from the narrowing of the spectrum. Usually it is assumed that the narrowing is given by a factor $1/\sqrt{N}$ (where N is the number of the coupled monomers) that is obtained e.g. for uncorrelated Gaussian static disorder.

Here we consider dynamic disorder and find, using numerical quantum calculations, for a non-Markovian environment a strongly enhanced narrowing of a factor $1/N$. On the other hand, for a Markovian environment it turns out that no narrowing at all occurs, showing that the narrowing strongly depends on the model assumed.

CPP 18.4 Tue 18:00 P1

Ultrafast dynamics of a new model bisporphyrin — •Martin Kullmann[1], Arthur Hipke[1], Patrick Nuernberger[1], Daniel C. G. Götz[2], Gerhard Bringmann[2], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg — [2]Institut für Organische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg

Porphyrins are attractive molecular systems because their tetrapyrrolic structure is similar to the light-harvesting chlorophyll which enables biomimetic applications like organic photovoltaic solar cells. The studies described in the present contribution offer insight into the photochemistry of an intrinsically axially chiral, directly β,β'-linked porphyrin dimer, bis[tetraphenylporphyrinato-zinc(II)] $(\mathrm{ZnTPP})_2$.

We present a comparative fs-resolved transient absorption study of $(\mathrm{ZnTPP})_2$ and its monomeric subunit ZnTPP after excitation to their respective first and second excited electronic state. In contrast to similar experiments on multiporphyrin systems which focused on a single time domain, often not extending over more than a few picoseconds, we provide a complete analysis on time scales ranging up to the nanosecond regime.

Results from global analysis schemes applied to both molecules will be presented. The monomer's relaxation process, which is in strong agreement with the literature, differs significantly from the dimer's kinetics. Preliminary interpretations based on this observation as well as on comparisons with similar literature-known compounds will be discussed.

CPP 18.5 Tue 18:00 P1

Single Molecule Studies of Calix[4]arene-linked Perylene Bisimide Dimers with Spectral and Temporal Resolution —

•Abey Issac[1], Dominique Ernst[1], Catharina Hippius[2], Frank Würthner[2], and Jürgen Köhler[1] — [1]Experimental Physics IV and Bayreuth Institute für Macromolecular Research (BIMF), University of Bayreuth, 95447 Bayreuth, Germany — [2]Institut für Organische Chemie and Röntgen Research Center for Complex Material Systems, Universität Würzburg, 97074 Würzburg, Germany

Initial studies of single calix[4]arene linked perylene bisimide dimers embedded in a polymer matrix revealed changes of the fluorescence intensity between high, medium and the background levels [1]. The change from the highest level to the background is associated with an efficient energy transfer between the two bisimide units. The medium intensity level presumably reflects the photoreduction of one of those units. Here we report about recent experiments where we recorded either the emission spectra or the fluorescence lifetime at different signal levels.

[1] D.Ernst, R.Hildner, C. Hippius, F. Würthner, J. Köhler, Chem.Phys.Lett. 482 (2009) 93

CPP 18.6 Tue 18:00 P1

Investigation of Electron Transfer in the Dye/Semiconductor Interface of Dye-Sensitized Zinc Oxide Nanoparticles

— •Kerstin Strauch[1,2,3], Christian Litwinski[2], Egmont Rohwer[3], Heinrich Schwoerer[3], Tebello Nyokong[2], and Derck Schlettwein[1] — [1]Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de — [2]Department of Chemistry, Rhodes University, Grahamstown, South Africa — [3]Laser Research Insitute, Physics Department, University of Stellenbosch, South Africa

As an alternative to dye-sensitized solar cells based on TiO_2 nanoparticles, electrodeposited ZnO was proposed as a porous, crystalline semiconductor matrix. However, until now considerably lower power conversion efficiencies were reported. A decreased injection efficiency from the excited state of the dye to the conduction band of the semiconductor was discussed as possible reason for this lower efficiency. As a model system, ZnO nanoparticles were used in order to allow a detailed time-resolved spectroscopic investigation. Different dye molecules were investigated as sensitizers for these nanoparticles. Time-correlated single photon counting (TCSPC) was used to determine the fluorescence lifetime of the dissolved sensitizer compared to the molecule bound to ZnO. In order to characterize details of the sensitizer excited state bound to ZnO femtosecond- transient absorption spectroscopy (fs-TAS) experiments were done. Implications for the technical application of the different sensitizers on ZnO are discussed.

CPP 18.7 Tue 18:00 P1

Quest for spatially correlated fluctuations in light-harvesting systems

— •Carsten Olbrich[1], Johan Strümpfer[2], Klaus Schulten[2], and Ulrich Kleinekathöfer[1] — [1]Jacobs University Bremen, Bremen, Germany — [2]University of Illinois, Urbana, USA

Photosynthesis is one of the essential mechanisms in nature to harvest energy for biochemical processes in plants and certain kinds of bacteria. Specific pigment-protein complexes, so-called light-harvesting (LH) complexes, have the function of absorbing light and transporting the energy to the photosynthetic reaction center. A few years back, experimental evidence has been reported for a coherent energy-transfer dynamics at 77 K in FMO. Based on molecular dynamics simulations at ambient temperatures, electronic structure calculations for the vertical excitation energies of the individual bacteriochlorophylls along the trajectory have been performed. Neither for the LH2 complex of *Rhodospirillum molischianum* nor for the FMO complex of the bacterium *Chlorobaculum tepidum* strong correlations have been found in the energy fluctuations [1,2]. In addition, the obtained data can be used to determine spectroscopic properties of the complexes [3].

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

[2] C. Olbrich, J. Strümpfer, K. Schulten, U. Kleinekathöfer, J. Phys. Chem. B. (in press).

[3] C. Olbrich, J. Liebers, U. Kleinekathöfer, phys. stat. sol. (b) (in press, DOI:10.1002/pssb.201000651).

CPP 18.8 Tue 18:00 P1

Comparing density matrix with ensemble-averaged wave packet dynamics

— •Mortaza Aghtar, Jörg Liebers, Carsten Olbrich, and Ulrich Kleinekathöfer — Jacobs University Bremen, Germany

In many physical, chemical and biological systems energy and charge transfer processes are of utmost importance. To determine the influence of the environment on these transport processes, equilibrium molecular dynamics simulations become more and more popular. In these simulations one usually determines the thermal fluctuations of certain energy gaps [1,2]. Those fluctuations are then either used to perform ensemble-averaged wave packet simulations directly [3] or to first determine a spectral density which in turn is used for density matrix calculations [1,2]. Here we compare these two latter approaches. In order to do so, we create artificial fluctuations corresponding to a fixed spectral density. Subsequently, density matrix and wave packet simulations are compared in a controlled manner for different parameter regimes.

[1] A. Damjanovc, I. Kosztin, U. Kleinekathöfer and K. Schulten, Phys. Rev. E 65, 031 919 (2002).

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

[3] C. Olbrich, J. Liebers, U. Kleinekathöfer, phys. stat. sol. (b) (in press, DOI:10.1002/pssb.201000651).

CPP 18.9 Tue 18:00 P1

Mapping the spin states of Fe(II) spin-crossover compounds by STM

— •Michael Stocker[1], Sven Besendörfer[1], Katja Student[2], Andreas Grohmann[2], and Paul Müller[1] — [1]Department of Physics and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Germany. — [2]Institut für Chemie, Technische Universität Berlin, Germany.

We present measurements of the spin state of Fe(II) spin-crossover (SCO) compounds by STM spectroscopy. The talk focuses on the investigation of $[FeL_2]^{2+}$ [L = 2,6-di(pyrazol-1-yl)pyridine]. Measurements of small clusters of the molecule deposited onto HOPG surfaces are shown and compared to the results of previous measurements of Fe(II) SCO compounds as well as measurements of a solely high-spin compound with a similar coordination motif[1]. The different spin states exhibit a strong contrast in the current maps of CITS measurements. At room temperature, a reversal of both spin states was observed on a timescale of minutes. We also found indications for a dependence of the spin state on the surface matching of the deposited clusters.

[1] M.S. Alam, M. Stocker, K. Gieb, P. Müller, M. Haryono, K. Student, A. Grohmann, Angew. Chem. Int. Ed. 49, 1159 (2010).

CPP 19: Poster: Interfaces and Thin Films

Time: Tuesday 18:00–20:00 Location: P2

CPP 19.1 Tue 18:00 P2

Kinetics of structural changes in lamellar poly(styrene-b-butadiene) diblock copolymer thin films during thermal treatment

— •Alessandro Sepe[1], Dorthe Posselt[2], Sebastian Jaksch[1], Eicke Tilo Hoppe[1], David Magerl[1], Qi Zhong[1], Jan Perlich[4], Detlef-Matthias Smilgies[3], and Christine M. Papadakis[1] — [1]TU München, Physikdepartment, Physik der weichen Materie, Garching, Germany — [2]Institute for Science, Systems and Models, Roskilde University, Denmark — [3]Cornell High-Energy Synchrotron Source (CHESS), Ithaca, U.S.A. — [4]HASYLAB at DESY, Hamburg

Nanostructured block copolymer thin films find a number of applications, especially for optical elements. 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 wish to elucidate the mechanisms of structural changes induced by thermal treatment. 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. The poly(styrene-b-butadiene) system studied by us is well-suited to address this question because it has initially the perpendicular lamellar orientation. 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 destruction of structure is observed.

CPP 19.2 Tue 18:00 P2

Strong segregation limit of a diblock copolymer film in an electric field — •Michael Harrach, Barbara Drossel, Marianne Heckmann, and Tiago de Paula Peixoto — Institut für Festkörperphysik, TU Darmstadt

We present an algorithm to evaluate the free energy of a thin film of diblock copolymers in an electric field at low temperatures. We apply the strong-segregation limit, where only one type of monomer is present in each domain. We assign different dielectric constants to the two types of domains. 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. We evaluate the different contributions to the free energy for different types of phases, with the goal to find the phase with the lowest free energy as a function of the film thickness and the applied electric field.

CPP 19.3 Tue 18:00 P2

Control of Lamella Orientation in Confined Block Copolymer Films — •Vanessa Weith, Alexei Krekhov, and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany

The study of phase separation in polymer blends offers substantial opportunities to control the morphology of the evolving patterns. This is of considerable fundamental and technological importance in order to develop new materials to achieve specific properties. New strategies to control the long-range order in the nanostructures formed by microphase separation in block copolymers can be developed with the help of recently found thickness-dependent lamella orientation in diblock copolymer films [1].

We have studied this issue using a mean-field approach. Investigating the existence, stability and free energy of lamellar solutions in infinite and confined geometries in one spatial dimension, the results agree with those of other models based on self-consistent field theory [2] or free energy [3]. Extending the analysis to two spatial dimensions helps to determine which orientation of the lamella is selected depending on the input parameters. Furthermore the dynamics of the spatio-temporal behavior of the phase separation process is characterized.

[1] V. Olszowka, L. Tsarkova, and A. Böker, Soft Matter 5, 812 (2009)

[2] M. W. Matsen, J. Chem. Phys. 106, 7781 (1997)

[3] D. G. Walton, G. J. Kellog, and A. M. Mayes, Macromolecules 27, 6225 (1994)

CPP 19.4 Tue 18:00 P2

Calorimetric investigations of thin films of micelles formed by triblockcopolymers — •Heiko Huth[1], Julia Gensel[2], Andreas Fery[2], and Christoph Schick[1] — [1]Universität Rostock, Institut für Physik, Wismarsche Straße 43-45, 18051 Rostock, Germany — [2]Universität Bayreuth Physikalische Chemie II, Universitätsstraße 30, 95440 Bayreuth, Germany

In the recent years investigations in the nano sized range is in the focus of many researchers. For basic understanding as well as for practical applications the behavior of thin films and other confinements in small dimensions is of interest.

As one example for applications there is the idea of structured thin films due to self assembly i.e. of complex substructures as micelles. While for structural investigations several methods for thin films are present it is difficult to find methods to observe dynamic properties. AC-chip calorimetry has demonstrated the ability to measure thin polymeric films [1] and is now used as a very sensitive tool for calorimetric investigations of thin films formed by micelles.

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

CPP 19.5 Tue 18:00 P2

Structure formation and dynamics of thin liquid crystal (8CB) films depending on the type of substrate — Benjamin Schulz[1,2], •Daniela Täuber[1], and Christian von Borczyskowski[1] — [1]nanoMA, TU-Chemnitz, Institut für Physik — [2]now at MPI-DS, Göttingen

Taylor made single dye molecules were used to study structure and dynamics within 220 nm thick liquid crystal films. While the diffusion is strongly heterogeneous for thin 8CB films [1] on Si wafers with native SiOx as well as with 100 nm thermally grown SiOx, the structure of the film differs: On 100 nm SiOx, the liquid crystal self-organizes into focal conic domains [2], while on native SiOx a terraced structure with holes is observed. Using dye molecules which align with the liquid crystal, a correlation between structure and dynamics is shown.

[1] B. Schulz, D. Täuber, F. Friedriszik, H. Graaf, J. Schuster and C. von Borczyskowski: PCCP 12 (2010) 11555

[2] V. Designolle, S. Herminghaus, T. Pfohl, und Ch. Bahr: Langmuir 22 (2006) 363

CPP 19.6 Tue 18:00 P2

Equilibrium geometry of three smectic liquid crystalline films — •Torsten Trittel[1], Ruth Aldred[2], and Ralf Stannarius[1] — [1]Otto-von-Guericke Universität, Institut für experimentelle Physik, 39106 Magdeburg — [2]The University of Exeter, School of Physics, Exeter EX4 4QL

We spotlight the geometrical properties of Plateau borders in an arrangement of connected fluid free standing films. In our experiment, a circular Plateau border surrounds a planar smectic film and connects it with two smectic catenoids. We show that similar to soap films, the geometry can be described by a negative line tension of the circular contact region. It is obvious that the equilibrium angle between the films depends upon the liquid content in the contact region, and with increasing liquid content, deviations from Plateau's rule are observed. The results are qualitatively comparable to soap films. A possible origin of slight quantitative differences is discussed.

CPP 19.7 Tue 18:00 P2

Interactions and stability of foam films from oppositely charged surfactant mixtures — •Heiko Fauser, Nora Kristen-Hochrein, Natascha Schelero, and Regine von Klitzing — Stranski-Laboratorium, Institut für Chemie TU-Berlin, Strasse des 17. Juni 124, 10623 Berlin, Deutschland

Mixtures of cationic and anionic surfactants are widely used in industrial processes and products. Until this date mainly the adsorption behavior of oppositely charged surfactants at liquid and solid surfaces has been investigated. In order to understand adsorption at foam films it is important to investigate free-standing foam films. A measurement of the interactions between two opposing foam-film interfaces is the disjoining pressure, which is considered to be the sum of repulsive electrostatic and steric forces, as well as attractive van der Waals forces. The disjoining pressure is measured with a so called Thin Film Pressure Balance.

Mixtures of oppositely charged surfactants tend to show interesting properties and behavior in terms of stability and thickness of the free-standing films. For example is the formation of a Common Black Film or a much thinner but more stable Newton Black Film governed by the concentration ratio of the surfactant mixture.

Also the question how supplement measurements of other physical properties like surface tension or surface rheology can support to understand our results and help to develop a more precise description of such surfactant mixtures is taken into account.

CPP 19.8 Tue 18:00 P2

Structures in molecular thin smectic liquid crystal films — •Benjamin Schulz and Christian Bahr — MPI for Dynamics and Self-Organization, Bunsenstraße 10, 37073 Göttingen

We present a convenient technique to create thin films of the smectic liquid crystal 8CB with a defined number of molecular layers on silicon surfaces. Using AFM- and ellipsometry-measurements we observe characteristic porous surface textures that are common to all films with a thickness of up to 5 layers. Even though those films show liquid-like mobility of the molecules, the structures turn out to remain stable on the time scales of days. Additionally, the properties of the films are studied when heated into the nematic and isotropic temperature range of the bulk material. For films with a thickness of only one smectic layer, a suppression of the nematic phase is observed, whereas the other films exhibit a shift of the phase transition temperature.

CPP 19.9 Tue 18:00 P2

Single Molecule Studies in Liquid Crystals — •Martin Pumpa and Frank Cichos — Molecular Nanophotonics Group, University of Leipzig

Liquid crystals show strong orientational order along a certain director, while lacking spatial order of their centers of mass. For uniaxial liquid crystals the orientational properties lead to anisotropy in the mobility and the optical properties of the material. Recent optical studies focus on their bulk behavior or the diffusion of microscopic particles, gaining only limited information on the microscopic dynamics in the liquid crystal. Single molecule fluorescence detection is in principle able to take a deeper look inside these systems, however, only few single molecule experiments have been published so far.

Here, we compare fluorescence depolarization experiments and single molecule tracking to get the anisotropic mobility of a fluorescent tracer molecule in LC samples. With polarization contrast images we are able to correlate findings from these experiments with the director orientation in the observed areas. Our results deviate strongly from recently published NMR results on the self-diffusion in liquid crystals. Thus we suggest based on additional FRAP measurements a strong influence of the fluorophore on the director structure in its immediate surrounding. This results in a smaller diffusion coefficient due to higher effective viscosities along and perpendicular to the macroscopic director orientation.

CPP 19.10 Tue 18:00 P2

A new method to characterize surface texture via observation of single molecules in video microscopy — •Mario Heidernätsch and Günter Radons — Chemnitz University of Technology, D-09126 Chemnitz, Germany

Single molecule video microscopy is a widely used tool to investigate the dynamic properties of thin liquid films. By analyzing the distribution of diffusivities [1], i.e. the local displacements obtained from the trajectories of the observed dyes, the influence of local inhomogeneities on the diffusion can be revealed. Especially in ultra-thin liquid films the local surface texture strongly influences the diffusivities, thus the resulting diffusion coefficient becomes spatial dependent. We present a new method, the so called diffusion map, which can be easily obtained either from the observed trajectories or, without the necessity of tracking, directly form the recorded videos. We can show that this diffusion map is an indirect representation of the surface texture.

[1] M. Bauer, M. Heidernätsch, D. Täuber, C. von Borczyskowski, G. Radons, Diffusion Fundamentals III **11** (2009), pp. 70.1-70.2

CPP 19.11 Tue 18:00 P2

Bio-chemical functionalization of silicon surfaces — •Lotta Römhildt[1], Claudia Kühn[1], Jörg Opitz[1,2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany — [2]Fraunhofer Institute IZFP Dresden, 01109 Dresden

Functionalization of the inorganic interface in nano-bio hybrid materials is a key step for a successful combination of silicon technology at the nanoscale with the specificity of biomolecular recognition in biological systems. The aims are to provide the desired functional groups for the covalent attachment of biomolecules, to guarantee the functionality of the bound biomolecules and to prevent unspecific attachment to the surface. Monolayers on silicon wafers were prepared by covalently binding organic molecules to the surface, such as organosilanes or alkenes, respectively. Biomolecules such as single-stranded DNA are acting as receptors for target molecules. They were further linked to this functionalized surface by using wet bio-chemistry. Static contact angle measurements for the quantification of the wetting behavior indicate that different molecular layers were successfully attached to silicon surfaces. The layer thickness and quality of the film formation were studied with ellipsometry and AFM. Functional end groups like the amino group and potential biomolecules such as DNA strands were labelled with fluorescent dyes to detect the binding with fluorescence microscopy.

CPP 19.12 Tue 18:00 P2

Atomistic Study of Substrate Effect on Polyelectrolyte Adsorption: Poly(Styrene Sulfonate) Monolayer — •Baofu Qiao, Juan Cerda, and Christian Holm — Institute for Computational Physics, University Stuttgart

All-atom level simulations are preformed to investigate the adsorption of polyelectrolytes, for the first time, onto different (hydrophobic vs. hydrophilic) adsorbing substrate, accompanied by a varied surface charge density. In the present work, poly(styrene sulfonate) (PSS) is employed. It shows that the exclusive presence of the short-range wall potential of van der Waals origin is strong enough to form a PSS adsorption layer. Two kinds of conformations of adsorbed PSS chains are observed. The "laying" PSS chains (flat adsorption layer) dominate, with some PSS chains "dangling" into the above solution, which is consistent with a previous experimental work (S. Block and C. A. Helm, J. Phys. Chem. B 2008, 112, 9318.).

CPP 19.13 Tue 18:00 P2

Impedance Spectroscopy Simulation of Solid Electrolytes — •Manuel Landstorfer[1,2], Stefan Funken[1], and Timo Jacob[2] — [1]Institut für Numerische Mathematik, Universität Ulm, Helmholtzstr. 18 — [2]Institut für Elektrochemie, Universität Ulm, Albert-Einstein-Allee 47

Solid electrolytes are promising functional materials for a wide range of applications, *e.g.* lithium ion batteries, solid oxide fuel cells, sensors or electrochromic devices. One of the main characterization methods of electrolytes is the impedance spectroscopy, in which the cell response to AC conditions is monitored. Besides the classical simulations of impedance spectroscopy, in which the electrolyte is modeled as a RC network, more fundamental studies in terms of transport equations can be performed.

We describe ion transport in a solid electrolyte via an extended Poisson–Nernst–Planck system, which takes into account the finite amount of ion sites. Boundary conditions for the impedance spectroscopy simulations are derived, which incorporate the capacitance of the electrode/electrolyte intermediate layer. It resolves space- and time-dependent the charge region within the solid electrolyte. Using a finite element method (FEM) and Newton's methods to solve the nonlinear partial differential equation system, we present numerical results for various frequencies allowing us to evaluate the system's response in impedance spectroscopy measurements. The AC frequency of purely capacitative behaviour, *i.e.* no double layer formation, is determined by our numerical studies.

CPP 19.14 Tue 18:00 P2

Biomineralisation 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], Christoph Sahle[1], Johannes Möller[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

Biomineralisation processes provide composite materials which show hierarchical organization as well as complex and controlled shapes. The biomineralisation processes in living organisms are controlled by proteins and the environment where the process takes place, e.g., the inner cell or the surface of membranes. We studied the biomineralisation 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 mineralisation process. The adsorption of iron oxide at the monolayers was observed by grazing incidence diffraction (GID) and extended x-ray absorption spectroscopy (EXAFS). The GID and EXAFS data show an agglomeration of iron oxides at the monolayers. The coordination of the forming iron oxides were similar to the coordination of lepidocrocite and goethite.

CPP 19.15 Tue 18:00 P2

Solvent mapping in conducting polymer blend films using Scanning Transmission X-ray Microscopy — •Markus Schindler[1], Robert Meier[1], Benjamin Watts[2], Jörg Raabe[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany — [2]Paul Scherrer Institute, 5232 Villigen, Switzerland

Since conducting polymers show widespread application possibilities, such as organic field effect transistors and solar cells, their long-time stability is moreover still a serious concern. Aging can be enhanced due to embedded solvent molecules retained in the polymer matrix of the thin films. The remaining solvent affects the mobility of the polymers leading to an ongoing change of the nanoscopic heterostructure, accompanied by changes in the electrical performance.

For thin conducting homopolymer films our results based on X-ray Spectroscopy show a strong dependence of the remaining solvent amount on the particular polymer-solvent-system. By using spatially resolving Scanning Transmission X-ray Microscopy not only compositional maps of polymer-blend films based on P3HT and PVK were obtained, but also solvent distribution maps revealing preferential domains depending on the majority component. This study is complemented with topology sensitive atomic force microscopy measurements.

CPP 19.16 Tue 18:00 P2

Low temperature sintering of thin film polymer/TiO2 solar cells — •Christoph Fahrenson[1], Sylvia Paul[1], Michael Schröder[3], Silvia Janietz[2], and Dieter Neher[1] — [1]Universität Potsdam — [2]Fraunhofer-Institut für Angewandte Polymerforschung, Golm — [3]Justus-Liebig-Universität Gießen

Hybrid solar cells combine an organic semiconductor with a suitable inorganic semiconductor (ref 1). In addition to studies on the well-known Grätzel cell, combinations of a dense or nanostructured TMO layer with soluble conjugated polymers have been subject to recent investigations. One of the problems in the development of efficient polymer/TiO2 cell is the sintering of TiO2-layer. In most cases, the TiO2 layer is prepared via the sol-gel technique and annealing at high temperatures is needed to transform the amorphous layer morphology into a crystalline nanoporous structure. We present a new method to prepare thin layers from crystalline titania nanoparticles while keeping the processing temperature below 100°C. Interlinkage between the individual TiO2 particle is enforced by illumination with UVC-light. Scanning electron microscope (SEM) is used to image the morphology of the thin nanoporous layers. Solar cells were built with the Titanium dioxide layers sintered at moderate temperatures or after UVC sintering, using different donor polymers. Initial experiments show that cells with UVC-sintered layers show comparable solar cell performances than devices using conventional titania layers.

1.*A. C. Arango, L. R. Johnson, et al., Advanced Materials, 12, (2000).

CPP 19.17 Tue 18:00 P2

Fabrication of metallic nanostructures for surface plasmon induced topography changes in azobenzene polymer films — •Arulmozhi Geetha Loganathan[1], Tobias König[1,2], Jürgen Rühe[1], and Svetlana Santer[2] — [1]Department of Microsystems Engineering (IMTEK), University of Freiburg — [2]Institute for Experimental Physics, University of Potsdam

We report on the construction of photosensitive polymer films with integrated metallic gratings in the form of nano-stripes. The metallic stripes were fabricated by two photon lithography. The procedure consist of two steps: First a polymer nano-structure is generated, followed by evaporation of a metallic layer on top of the nano-pattern. Subsequently, thin photosensitive azopolymer films are deposited on top of the active metallic elements. The metallic structures act as nano-scale antennas, in which surface plasmons are excited during homogeneous irradiation with light of an appropriate wavelength. During irradiation of the surface with homogeneous UV light complex intensity patterns can be excited at the metallic interface. The size of generated intensity pattern is below the diffraction limit and can be adjusted under the influence of external stimuli such as variations of the polarization and/or wavelength of the incoming light. The distribution of surface plasmons can be predicted by using FDTD simulations and compared with experimental results. The evanescent field of the surface plasmons is used to induce topography changes in the azobenzene polymer films.

CPP 19.18 Tue 18:00 P2

Novel structuring routine of PEDOT:PSS applied to organic photovoltaics — •Christopher Birkenstock, Robert Meier, and Peter Müller-Buschbaum — TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany

In order to improve device characteristics in organic photovoltaic, nano- and micro-structured substrates and polymer layers show a promising way to increase efficiency by optimization of light harvesting and charge carrier separation in solar cells. In this work we present a novel micro-structuring method based on wet-imprinting principles, which can be applied on an electron blocking PEDOT:PSS layer as they are used in electronic applications. It is based on different microchannel polycarbonate molds and it allows a high ratio of reproducibility and an accurate control of the total film-thickness. The influence of the structuring of PEDOT:PSS on the optical absorption and the overall device efficiency for polymeric solar cells based on P3HT:F8BT blends is investigated. The inner film morphology and the surface topography of the blend films are probed. A light trapping effect is obtained, which allows thinner design conceptions and is interesting for better electrical conductivity trough the photoactive film.

CPP 19.19 Tue 18:00 P2

Surface shear viscosity measurements in quasi 2-d systems — •Uli Langer and Thomas M. Fischer — EP V, Uni Bayreuth, Germany

Measuring the surface shear viscosity of monolayers is a very sensitive way of observing changes in the ordering of the particles the monolayers consits of. Due to the high sensitivity of this method one even gets reliable values for the surface shear viscosity of monolayers in the liquid expanded phase. In contrary to passive microrheology where sensitivity is proportional to the time used for measuring, the measurements with active microrheology take less than a minute.

CPP 19.20 Tue 18:00 P2

Sub-microscopic changes in COP surface properties due to different surface activation processes — •Martin Laher and Sabine Hild — Department of Polymer Science, Johannes Kepler University Linz, Altenbergerstrasse 69, 4040 Linz

Even though the ongoing demand to substitute different materials for polymers due to low cost and mass producibility encouraged lots of studies in polymer science, several questions are still unsolved. A major concern of research is to understand, improve and adjust material properties for specific applications. The substitution of glass or mica with polymers for biological application involves the disadvantage of low surface energy of polymers. The motivation for surface treatments is to adjust surface properties required to improve bonding processes with other polymers. Changes caused by different types of surface modification can increase the surface energy of nonpolar polymers or decrease the glass transition. Due to plasma activation or solvent treatment processes, modifications of mechanical properties like adhesion, stiffness or Young*s modulus of cyclo-olefin-polymer (COP) are expected as well as changes in the microstructure and the hydrophobicity. Surface characterization by means of SFM techniques such as force-distance measurements and SFM-Nanoindentation testing are to be sensitive tools to investigate changes in mechanical properties of polymeric materials. The main challenge is to approve the applicability of provided sensitivity ranges of these methods to detect surface treatment induced changes in the nanometer surface range. Therefore, surface properties of COP samples have been investigated.

CPP 19.21 Tue 18:00 P2

The structure of the interface between a solid substrate and a supercritical gas — •Sebastian Holz, Julia Nase, Michael Paulus, and Metin Tolan — Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund

Adsorption at interfaces is critical for many processes in nature, e. g. 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. However, the interface with a possible restructuration of the supercritical molecules has never been directly measured. In particular, the exact density profile along the surface normal can be determined by x-ray reflectometry, a reliable and well adapted technique to determine the thickness and roughness of interfaces.

We report on preliminary results concerning the adsorption of supercritical carbon dioxide and methane on a silicium wafer. The critical point of carbon dioxide is at T = 304,1 K and p = 73,8 bar and of methane at T = 190,6 K and p = 46,1 bar. We present a new measurement environment meeting the demands of this experimentally difficult study.

CPP 19.22 Tue 18:00 P2

The mesoscopic structure of liquid–vapour interfaces — •Felix Höfling and Siegfried Dietrich — Max-Planck-Institut für Metallforschung, 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 the phenomenological capillary wave theory (CWT). Deviations from CWT 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.

We have performed extensive molecular dynamics simulations for a simple liquid of up to one million particles interacting via a truncated Lennard–Jones potential. Macroscopic properties such as the interface width and the surface tension have been determined and their dependence on system size and cutoff radius of the potential is discussed. Further, the interface structure as encoded in the position-dependent density-density correlation function $H(z_1, z_2, k)$ is analysed. A factorisation property is tested on the obtained data and the wavenumber-dependent surface tension is extracted. Finally, we will address consequences of an external gravitational field on the interface structure.

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

CPP 19.23 Tue 18:00 P2

Mesoscopic simulation of multiphase fluid dynamics: interfacial phenomena at pore scale — •Marta S. de La Lama, Stephan Herminghaus, and Martin Brinkmann — Max-Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany

The wide range of length scales involved in multiphase flow points to mesoscale algorithms that capture the relevant physics and coarse-grain the irrelevant atomistic details. The term Multiparticle Collision Dynamics (MPC) comprises a variety of particle-based algorithms which employ successive free-streaming and local multi-particle collision steps [1]. Such collisions are carried out by performing rotations of particle velocities in predetermined cells in a manner that conserves mass, momentum and energy.

The algorithm can be adapted for modeling of multicomponent mixtures [2], and we employ it to analyze interfacial phenomena at pore scale. For instance, we can vary the wetting conditions in slit-pores or observe the effect of heterogeneous wettability on capillary imbibition. Furthermore, MPC is well-suited for complex geometries and, on the other hand, it accounts for thermal fluctuations. This gives us the chance of dealing with more realistic systems. For instance, we analyze how capillary bridges may affect the flow in poly-disperse mesoscopic porous media, what could help to elucidate and optimize the underlying mechanisms that take place in oil-reservoirs and filter materials.

References: [1] G. Gompper et al. ,Adv. Polym. Sci. 221 ,1 (2009) [2] Y. Inoue et al. ,J. Comp. Phys. 201 ,191 (2004)

CPP 19.24 Tue 18:00 P2

The determination of intrinsic interfacial molecules — •Sofia Kantorovich[1,2], Marcello Sega[1], and Pal Jedlovszky[3] — [1]ICP, Universität Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart Germany — [2]USU, Lenin av. 51, Ekaterinburg, 620000 Russia — [3]EKF Department of Chemistry, H-3300 Eger, Leanyka u. 6, Hungary

The identification of molecules or atoms belonging to an interface has been a task of primary importance in many fields, from the case of single molecules to that of liquid-vapor and liquid-liquid interfaces. In the work of Jorge et al. [M. Jorge et al., J. Phys. Chem. C 2010] a comparative analysis showed that the ITIM algorithm [L.B. Partay et al., J. Comput. Chem. 2008], based on a ray-tracing approach, is nowadays the best compromise between speed and accuracy. All the method investigated share the drawback of being primarily developed for the analysis of planar-like liquid-liquid or liquid-vapor interfaces. Here we adopt the concept of weighted alpha-shapes as a tool for identifying interfacial molecules between different phases, independently on the geometry of the interface. We investigate the applicability and computational performances of this approach, and the possibility of its implementation in periodic boundary conditions. Examples of molecular systems with different geometry (planar, spherical and cylindrical) are shown, and in the case of planar interfaces, we provide comparison to the ITIM method. This findings of the study might be used to analyze the interfaces and interfacial properties of systems of physical, chemical and biological interest at different scales.

CPP 20: Poster: Computational Soft Matter Physics

Time: Tuesday 18:00–20:00 Location: P2

CPP 20.1 Tue 18:00 P2

Solvent effects on linear polymer chains - A Monte Carlo Study — •Christoph Jentzsch[1,2] and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Germany — [2]TU-Dresden, Intitut für theoretische Pyhsik, Germany

In Computer simulations the solvent is usually introduced implicitly by effective attraction between the monomers to reduce computational time. Strong monomer-monomer attractions such as necessary to simulate chain collaps lead to artefacts both in lattice and off-lattice models. Using a high-performance implementation of the Bond-Fluctuation-Method solvent particles can be explicitly taken into account. This allows us to study effects of poor solvent and collapse transitions of individual chains both statically and dynamically. We present results for single polymer chains under thermal solvent conditions as well as the effect of an external force on the conformation statistics of individual chains.

CPP 20.2 Tue 18:00 P2

Parallel Monte Carlo simulation of lattice polymers on graphics processing units — •Marco Werner[1,2] and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Germany — [2]Technische Universität Dresden - Institut für Theoretische Physik

A parallel version of the bond fluctuation model (BFM) was developed for programmable graphics processing units (GPUs). The BFM is a lattice-based dynamical Monte Carlo method addressing the universal dynamic and static properties of polymer structures [I. Carmesin, K. Kremer, Macromolecules, 21, 2819, (1988)]. Recent developments by graphic card industry give rise to new possibilities in terms of system size and simulation speed accessible by the BFM. Modern GPUs provide several hundreds of parallel processors which work most efficient with massively parallel processes. We make use of this architecture by associating each monomer to one parallel process. In one elementary step all monomers are tried to move simultaneously. Hereby, the number of random memory accesses is reduced and the rate of tried moves per monomer increases with increasing number of monomers. The statics and dynamics of samples like polymer melts are compared between parallel and serial BFM-code to ensure the equivalence both methods. On the latest generation of GPU we obtain a maximum up-speed of about 50 compared to actual serial processors.

CPP 20.3 Tue 18:00 P2

Possibility of Coherent Delocalized Nuclear Quantum States of Protons in Li_2NH — •Ole Schütt[1], Guillermo A. Ludueña[2], and Daniel Sebastiani[1] — [1]Physics Department, Freie Universität Berlin, Arnimallee 14, 141965 Berlin, Germany — [2]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany

We analyze the possibility of quantum delocalization in lithium imide (Li_2NH) in the condensed phase using ab initio path-integral molecular dynamics. Our results provide evidence that the effective potential felt by the protons in the material has a toroidal shape. The virtually flat potential may lead to quantum delocalization of the NH protons over the torus.

CPP 20.4 Tue 18:00 P2

Stochastic optimization of capping potentials for mixed QM/MM calculations — •Christoph Schiffmann and Daniel Sebastiani — Freie Universität Berlin, Institut für Theoretische Physik, Arnimallee 14, 14195 Berlin

We present a stochastic scheme to design & optimize capping potentials for use at the QM/MM boundary in mixed *ab initio*-classical calculations. In our scheme, the terminal atoms in the quantum subsystem are replaced by optimized capping pseudopotentials. Our aim is to minimize the perturbations in the electronic structure due to the cleaving of covalent bonds across the QM/MM boundary.
Komin, S.; Sebastiani, D. *JCTC* **2009**, 5, 1490-1498

Schiffmann C.; Sebastiani D. (*submitted*)

CPP 20.5 Tue 18:00 P2

Friction contribution to water-bond breakage kinetics — •Yann von Hansen[1], Felix Sedlmeier[1], Michael Hinczewski[1,2], and Roland R. Netz[1] — [1]Physik Department, Technische Universität München, 85748 Garching, Germany — [2]Institute for Physical Science and Technology, University of Maryland, College Park, MD 20742, USA

Based on separation trajectories 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 Fokker-Planck equation allows us to derive the diffusivity profile along the separation coordinate and thus to unambiguously disentangle the effects of free energy and local friction on the separation kinetics. For tightly coordinated water the friction is six times higher than in bulk, which can be interpreted in terms of a dominant reaction path that involves additional orthogonal coordinates.

CPP 21: Poster: Confinement of Polymers in Nanoscopic Layers - How Much do Properties Change?

Time: Tuesday 18:00–20:00 Location: P2

CPP 21.1 Tue 18:00 P2

Glassy dynamics of polymers in thin films and monomolecular layers — •Martin Tress[1], Emmanuel Mapesa[1], Anatoli Serghei[2], and Friedrich Kremer[1] — [1]Universität Leipzig, Leipzig — [2]Université Lyon 1, Villeurbanne, France

The glassy dynamics of nanometer thin polymer layers supported on a solid substrate was investigated by Braodband Dielectric Spectroscopy (BDS). The thickness was systematically reduced finally resulting in randomly distributed polymer coils. Highest priority was put on an appropriate sample preparation including an annealing procedure for sufficient long time at elevated temperatures in inert atmosphere to avoid effects due to remaining solvent and chemical degradation. Further, detailed checks of the surface topology by atomic force microscopy (AFM) were performed to verify stability of the samples during the whole measurement. The dynamics is compared to the bulk to trace changes due to the impact of the interface and to give a length scale for the interfacial interactions.

CPP 21.2 Tue 18:00 P2

Glassy dynamics of ultra-thin layers of polyisoprene — •Emmanuel Mapesa, Martin Tress, and Friedrich Kremer — Universität Leipzig, Leipzig

Broadband Dielectric Spectroscopy (BDS) - in combination with a nanostructured electrode arrangement - is used to study thin layers of polyisoprene. In the view of BDS, polyisoprene 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. These fraction adds up to one dipole moment of the whole polymer chain corresponding to the end-to-end vector of the molecule. This enables the investigation of two distinct relaxation modes taking place at two different length scales: the segmental motion which involves structures of about 1 nm in size (2 to 3 monomer units) and the so-called normal mode which represents the dynamics of the whole macromolecule. By making measurements on identical samples in capped and uncapped geometries, and systematically reducing the layer thicknesses, we show clearly the changes that occur in these two relaxation processes due to the presence of a solid interface. Special attention is given to sample preparation and treatment.

CPP 21.3 Tue 18:00 P2

Dynamic 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

The dynamic glass transition (α relaxation) of thin poly(bisphenol A carbonate) films (down to 10 nm) capped between two aluminum electrodes is investigated by dielectric relaxation spectroscopy. There is no thickness (polymeric layer) dependence of the dynamic glass transition temperature down to a critical thickness of 20 nm. For thickness below ~ 20 nm, an increase of dynamic glass transition temperature is observed. The Vogel-Fulcher-Tammann (VFT) equation is further applied to fit the data of relaxation rate vs dynamic glass transition temperature which reveals that the Vogel temperature increases with decreasing film thickness d. These peculiar properties are discussed in terms of the formation of a top layer of adsorbed poly(bisphenol A carbonate) segments having a reduced molecular mobility with regard to bulk poly(bisphenol A carbonate) at the experimental time scale. Contact angle measurement is performed to confirm the strong interaction between the aluminum layer and poly(bisphenol A carbonate). The interfacial energy between them is calculated to be 3.1 mJ/m2 which is related to an increase of dynamic glass transition temperature.

CPP 21.4 Tue 18:00 P2

Calorimetric 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

The differential alternating current chip calorimeter with the sensitivity of a few tens of pJ/K was applied to study the glass transition of thin poly(bisphenol A carbonate) films with thickness ranging from 35 nm to 230 nm. The temperature dependent measurement (393.15-463.15 K) of complex heat capacity of nanometer-thin films was carried out in the frequency range typically from 1 Hz to 1000 Hz. Amplitude and phase angle of the complex differential voltage as a function of the temperature, respectively, were attained in the measurement, which can be used to determine the calorimetric glass transition temperature. No thickness dependency of calorimetric glass transition temperature was observed within an uncertainty of +/-3 K at every setting frequency. The frequency dependence of calorimetric glass transition temperatures was further analyzed by the fitting of Vogel-Fulcher-Tammann (VFT) equation. It is shown that there is no deviation from the common VFT behavior.

CPP 21.5 Tue 18:00 P2

Structure-Property Relationships of Plasma Deposited Poly (acrylic acid) Thin Films — •Alaa Fahmy, Renate Mix, Andreas Schönhals, and Jörg Friedrich — BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany

Poly (acrylic acid) films with a thickness of about 150 nm were deposited in the pulsed plasma regime onto aluminium and glass substrates. The structure/property relationships of these samples were studied in dependence on the duty cycle (DC) of the plasma by a broad combination of different techniques and probes. For the first time volume sensitive methods (FTIR, dielectric spectroscopy, and differential scanning calorimetry) are combined with surface analytics by employing XPS. For an unambiguous identification of COOH groups by XPS, derivatisation with trifluoroethanol was accomplished. Quantitative FTIR investigations give qualitatively the same dependence of the concentration of COOH groups on DC like XPS investigations. The dielectric measurements reveal that the structure of the plasma deposited films is different from that of the bulk material. Especially a lower glass transition temperature is observed. This result points to a highly branched structure of the plasma deposited polymer with a high number of dangling chains. Moreover, the dielectric measurements show that the plasma deposited films are not thermally stable but undergo a post plasma chemical reaction during heating, where the reaction kinetics depends on DC.

CPP 21.6 Tue 18:00 P2

Form factor of polymer melts: Deviations from ideal Gaussian behavior — •Julia Zabel[1], Caleb Dyer[2], Mark Dadmun[2], Hendrik Meyer[1], Joachim Wittmer[1], and Joerg Baschnagel[1] — [1]Insitut Charles Sadron, CNRS, 23 rue du Loess, 67037 Strasbourg, France — [2]Univ Tennessee, Dept Chem, Knoxville, TN 37996 USA

With a disarmingly simple argument Flory predicted that a flexible polymer in a melt behaves as an ideal, 3 dimensional random walk, its step length Gaussian distributed. This hypothesis is based on excluded volume screening in a dense melt. The Gaussian coil gives rise to such important scaling laws as $R_g \sim N^{1/2}$ which are fundamental in modern polymer physics. Over the last decade the Flory hypothesis has been revisited and corrections suggested [Semenov et al, Euro Phys. J. E, 12 (2003)]. Coarse grained simulation mod- els support these corrections [Wittmer et al, EPL, 77 (2007)]. Most recently small angle neutron scattering experiments have been performed on high molecular weight PIB and PDMS melts. The results will be presented here and their deviations from ideal behavior discussed.

CPP 21.7 Tue 18:00 P2

Effect of substrate on the formation of polyelectrolytes multilayers — •Maximilian Zerball, Samantha Micciulla, Chloé Chevigny, and Regine von Klitzing — Stranski-Lab., TU Berlin, Institut für Chemie, Sekr. TC 9, 10623 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 opened the door for a wide variety of potential applications for polyelectrolyte multilayers (PEM), for example chemical reactors, antireflective coatings, containers or filtration membranes. 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 this deposition is still missing: this poster will present results which focus on the influence of the substrate on the formation of the multilayers. For this purpose different substrates are studied: by directly changing the nature of the substrate (Silicon or Gold), but also by chemically modifying 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, both either with long or short chain lengths. The thickness, roughness and aspect of the PEM are monitored as a function of the number of layers deposited by a complementary use of ellipsometry (with humidity control) and AFM. We can then very finely determine the substrate influence zone, and what the vicinity to the substrate changes inside this zone.

CPP 21.8 Tue 18:00 P2

Fluidics of confined liquid films: Impact of slippage on spinodal dewetting — •Matthias Lessel, Oliver Bäumchen, Sabrina Häfner, and Karin Jacobs — Department of Experimental Physics, Saarland University, D-66041 Saarbrücken, Germany

We investigate the dewetting dynamics of short-chained polystyrene (PS) films with thicknesses in the range of a few nanometers. According to the stability criteria derived from the effective interface potential, capillary waves are amplified and cause film thickness variations, a scenario termed spinodal dewetting. By in situ AFM investigations, the dynamics of spinodal dewetting is quantified [1, 2]. Due to confinement of the polymer in a thin film, physical properties such as the glass transition temperature change compared to the bulk properties. Recently, Yang et al. [3] were able to provide evidence for a highly mobile surface layer at the air/liquid interface of unentangled PS films. Bäumchen et al. showed for entangled PS films that the inter-chain entaglement density is reduced close to the interface [4]. An interfacial layer is capable to influence significantly the flow dynamics of the polymer. Polymer dewetting is studied by using substrates with different hydrophobic coatings like self-assembled monolayers of silanes or an amorphous fluoropolymer (AF 1600) coating.

[1] R. Seemann et al., Phys. Rev. Lett., 86 (2001), 5534.
[2] R. Fetzer et al., Phys. Rev. Lett., 99 (2007), 114503.
[3] Z. Yang et al., Science, 328 (2010), 1676.
[4] O. Bäumchen et al., Phys. Rev. Lett. 103 (2009) 247801.

CPP 22: Poster: Glass Transition and Dynamics of Liquids

Time: Tuesday 18:00–20:00 Location: P2

CPP 22.1 Tue 18:00 P2

Elastic Properties of Glasses — •Christian L. Klix, Florian Ebert, Georg Maret, and Peter Keim — University of Konstanz, D-78457 Konstanz, Germany

In this contribution, we present experimental results on the elastic properties of a two dimensional colloidal glass former. Given that glasses are solids, they exhibit a mechanical behaviour similar to crystals, i.e. they possess a finite shear modulus μ. We first extract the dispersion relation of the system where data hinting at structural change in the glassy state is found. Next, this dispersion relation is used to derive the moduli from modes in the long wavelength limit which are thermally excited [1]. 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 lets us determine the glass transition temperature T_g precisely.

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

CPP 22.2 Tue 18:00 P2

Low-Temperature Dynamics in Amorphous Polymers and Low-Molecular-Weight Glasses — Study with Single-Molecule Spectroscopy — Ivan Yu. Eremchev[1], Yury G. Vainer[1], Andrei V. Naumov[1], and •Lothar Kador[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

The dynamics in several low-molecular-weight glasses and in amorphous polyisobutylene of different molecular weights is investigated with single-molecule spectroscopy at temperatures of 4.5 and 7 K. Surprisingly, only the polymers with long chain lengths follow the prediction of the standard tunneling model and feature spectral jumps of the single-molecule lines between a small number of well-defined frequency positions corresponding to the coupling to few isolated tunneling systems. Glasses consisting of smaller molecules and oligomers show much richer dynamics: In most of them the spectral diffusion is so fast that single-molecule spectra can hardly or not at all be recorded and only irregular fluorescence flares are detected. Hence, the low-temperature dynamics of disordered solids is not universal but depends on the structure and chemical composition of the material. In polyisobutylene, the transition from small-molecule-like to polymer-like behavior occurs at chain lengths of a few hundred repeat units.

CPP 22.3 Tue 18:00 P2

Shear relaxation of simulated glass-forming polymer melts — •Stephan Frey[1], Hendrik Meyer[1], Joerg Baschnagel[1], and Matthias Fuchs[2] — [1]Institut Charles Sadron, F-67034 Strasbourg, France — [2]University of Konstanz, D-78457 Konstanz, Germany

Approaching the glass transition polymer melts show a remarkable increase of their viscosity by many orders of magnitude. The aim of this study is to gain a deeper insight into the processes which are involved in this phenomenon. We simulate polymer melts using a generic bead-spring model in which polymers are modeled as flexible chains. During long simulation runs the polymer melt is cooled down towards the glass transition temperature. The present work builds upon previous work which was focussed on the scattering function and related quantities. Here we concentrate on current correlation functions and connected quantities which are analyzed as a function of temperature, chain length and system size.

CPP 22.4 Tue 18:00 P2

Molecular relaxation processes in a MOF-5 structure revealed by broadband dielectric spectroscopy: signature of phenylene ring fluctuations — Stefan Frunza[1], •Andreas Schönhals[2], Ligia Frunza[1], Paul Ganea[1], Hendrik Kosslick[3], Jörg Harloff[4], and Axel Schulz[3] — [1]National Institute of Materials Physics, R-077125 Magurele, Romania — [2]BAM Federal Institute for Materials Research and Testing, D-12205 Berlin, Germany — [3]Leibnitz Institute for Catalysis at the University of Rostock, D-18059 Rostock, Germany — [4]University of Rostock, Institute of Chemistry, D-18059 Rostock, Germany

The molecular mobility of a MOF-5 metal-organic framework was investigated by broadband dielectric spectroscopy. Three relaxation processes were revealed. The temperature dependence of their relaxation rates follows an Arrhenius law. The process observed at lower temperatures is attributed to bending fluctuations of the edges of the cages involving the Zn-O clusters. The processes (*region II*) at higher temperatures were assigned to fluctuations of phenyl rings in agreement with the NMR data found by Gould et al. [J. Am. Chem. Soc. 2008, 130, 3246]. The carboxylate groups might be also involved. The rotational fluctuations of the phenyl rings leading to the low frequency part of relaxation region II might be hindered either by some solvent molecules entrapped in the cages or by an interpenetrated structure and have a broad distribution of activation energies. The high frequency part of region II corresponds nearly to a Debye-like process: This is explained by a well-defined structure of empty pores.

CPP 22.5 Tue 18:00 P2

Molecular dynamics of glass forming liquids under geometrical nano-confinement — •Wycliffe Kipnusu[1], Ciprian Iacob[1], Joshua Sangoro[1], Roger Gläser[2], and Friedrich Kremer[1] — [1]Institute of Experimental Physics I, University of Leipzig, Leipzig, Germany — [2]Institute of Chemical Technology, University of Leipzig, Leipzig, Germany

Translational and rotational dynamics in glass forming liquids confined in porous silica membranes having parallel cylindrical pores with diameters ranging between 5-12nm is studied by Broadband Dielectric Spectroscopy (BDS). Molecular dynamics, as reflected on the microscopic scale by the rotational and translation diffusion, exhibit deviations from the bulk behaviour when glass forming liquids are under mesoscopic confinement. The deviation is a result of interplay between surface effects due to interaction of the molecules with the pore walls and confinement effects pressumably caused by a change in packing density of the constrained molecules.

References:

[1]C. Iacob et al., Phys.Chem.Chem.Phys.11, 913-916, (2010).

[2]J. Sangoro et al., Phys.Chem.Chem.Phys. 12, 13798-13803, (2009).

CPP 22.6 Tue 18:00 P2

Dielectric relaxation of a nematic liquid crystal dispersed in a polar or non-polar polymer matrix — Lakshmi Meena Ganesan, •Lars Holländer, Werner Wirges, Peter Frübing, and Reimund Gerhard — Universität Potsdam

Polymer-dispersed liquid-crystal (PDLC) films were prepared from a nematic liquid crystal (LC) and polar poly(vinylidene fluoride-trifluoroethylene) (P(VDF-TrFE)) or non-polar poly(methyl methacrylate) (PMMA) as polymer matrix materials. During the preparation process, micrometer-sized droplets of LC are formed inside the polymer matrices.

The influence of the polymer matrix on the dielectric behavior of the LC was investigated by means of dielectric relaxation spectroscopy. From activation-energy calculations, it is assumed that the LC in the center of the droplets behaves like bulk material. Nevertheless, the angular motions of the dipole moments of the nematogen are slowed down in PDLC films by interfacial effects. This hindrance in motion is more pronounced in samples of polar P(VDF-TrFE) than in samples of non-polar PMMA and indicates a stronger interaction between the liquid-crystal molecules and the polar polymer molecules.

CPP 22.7 Tue 18:00 P2

Confinement-induced glass transition of n-butanol in silicon-nanochannels — •Carsten Biehl, Rene Berwanger, and Rolf Pelster — FR 7.2 Experimentalphysik, Universität des Saarlandes, D-66123 Saarbrücken, Germany

We have investigated the molecular dynamics of n-butanol, C_4H_9OH, confined in mesoporous silicon oxide with a mean pore radius of 7 nm. In contrast to the bulk material, confined butanol does not crystallize upon slow cooling. Using dielectric spectroscopy we observe a glass transition and determine the glass transition temperature T_g. Upon slow heating we observe indications for a partial crystallization in the temperature range above 125 K. We compare these results to measurements on quenched bulk butanol showing the formation of a metastable glacial state as a result of a frustrated crystallization process [1,2].

[1] I. M. Shmyt'ko. R. J. Jiménez-Riobóo, M. Hassaine and A. A. Ramos, J. Phys.: Condens. Matter 22, 195102 (2010)

[2] M. Hassaine et al, J. Chem. Phys. 131, 174508 (2009)

CPP 22.8 Tue 18:00 P2

Investigation of discotic liquid crystals — •Christina Krause, Huajie Yin, and Andreas Schönhals — BAM, Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany

Broadband Dielectric Spectroscopy is applied in a broad frequency ($10^{-1} - 10^9$ Hz) and temperature range (173-283 K) to study the discotic liquid crystal Pyrene-1,3,6,8-tetracarboxylic tetra(2-ethylhexyl)esther, 2,3,6,7,10,11 Hexakis(pentyloxy)triphenylene and 2,3,6,7,10,11-Hexakis(hexyloxy)triphenylene in the bulk state. The temperature dependence of the relaxation rates of Pyrene-1,3,6,8-tetracarboxylic tetra(2-ethylhexyl)esther and 2,3,6,7,10,11-Hexakis(hexyloxy)triphenylene in the lower temperature range might be described by the Vogel-Fulcher-Tamann equation. For 2,3,6,7,10,11-Hexakis(pentyloxy)triphenylene the relaxation process in the lower temperature range shows an Arrhenius-type temperature dependence. To obtain an extensive understanding of the underlying processes Differential Scanning Calorimetry and Alternating Chip Calorimetry are performed. Investigations of Pyrene-1,3,6,8-tetracarboxylic tetra(2-ethylhexyl)esther confined to porous silicon membranes and similar measurements of other discotic liquid crystals will be carried out in the future.

CPP 22.9 Tue 18:00 P2

Perfluorinated surfactants as model charged systems for understanding the effect of confinement on proton transport and water mobility in fuel cell membranes. A study by QENS — Sandrine Lyonnard[1], Quentin Berrod[1], •Beate-Annette Brüning[1], Gerard Gebel[1], Armel Guillermo[1], Hossein Ftouni[1], Jacques Ollivier[2], and Bernhard Frick[2] — [1]CEA, INAC/SPrAM/PCI, UMR 5819, 17 Av. des Martyrs, 38000 Grenoble, France — [2]Institut Laue-Langevin,6 rue Jules Horowitz,38042 Grenoble,France

We have investigated the dynamical properties of water confined in mesomorphous phases of perfluorinated sulfonic surfactants [1]. These systems mimic the physico-chemical properties of the perfluorinated Nafion membranes which are used as electrolyte in fuel cells. As the surfactants offer the advantage to self-assemble in well defined organized phases (e. g. hexagonal, lamellar), they are used as model charged systems to understand the structure transport relationship in complex real materials. Geometry and typical confinement size can be tuned through water concentration and temperature. A QENS study on hexagonal and lamellar phases was performed on both time-of-flight and backscattering spectrometers, covering a dynamic range from pico-to nanoseconds. Analysis of the data with localized translational diffusion models shows the existence of a strong confinement effect that depends on geometry. Typical confinement sizes and diffusion coefficients are obtained and compared to Nafion.

[1] S. Lyonnard et al., Eur. Phys. J ST 189, 205-216 (2010).

CPP 23: Poster: Semicrystalline Polymers, Polymer Crystallization and Self-Assembly

Time: Tuesday 18:00–20:00 Location: P2

CPP 23.1 Tue 18:00 P2

Deformationsverhalten einzelner kristalliner Lamellen in elastomerem Polypropylen: Verbiegung, Dehnung und Fragmentation — Mechthild Franke und •Robert Magerle — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

Elastomeres Polypropylen (ePP) zeichnet sich durch einen sehr niedrigen Anteil kristalliner Bereiche aus (10 bis 25%), die als einzelne kristalline Lamellen sowie in Verbünden von Lamellen in einer Matrix von amorphem Polypropylen vorliegen. Wir untersuchen das Deformationsverhalten dieser komplexen Gefügestruktur mit einem in ein Rasterkraftmikroskop integrierten Mikrozugversuch. Freitragende, nur wenige Mikrometer dicke ePP-Filme können damit kontrolliert gedehnt und wieder relaxiert werden; gleichzeitig können Veränderungen der Gefügestruktur an der Oberfläche der Filme mittels Rasterkraftmikroskopie abgebildet werden. Unsere Bildreihen zeigen eine Vielzahl unterschiedlicher Deformationsprozesse kristalliner Lamellen: Verbiegung und Dehnung einzelner Lamellen, Bildung von Knicken bei Dehnung, sowie das Auseinanderbrechen einzelner kristalliner Lamellen in etwa 15 nm große Blöcke. Verzweigungen zwischen Lamellen und epitakitsch darauf gewachsene Tochterlamellen weisen beim Dehnen feste Winkel auf, was zu lokal auxetischem Verhalten einzelner Lamellenverbünde führen kann. Das beobachtete Deformationsverhalten kann sehr gut mit einem Block- und Dehnfugenmodell der kristallinen Lamellen erklärt werden.

CPP 23.2 Tue 18:00 P2

Interplay between semicrystalline microstructure and viscoelastic properties of elastomeric polypropylenes — •Martin Neumann and Robert Magerle — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

We aim at understanding how mechanical stress relaxation is affected by the heterogeneous microstructure of semicrystalline polymers. As a model system we study elastomeric polypropylenes (ePP) with different degrees of crystallinity and different molecular weights. Further control about the microstructure and the entanglement density is provided by the annealing temperature and time. With a microtensile testing setup integrated in a scanning force microscope (SFM) we study the nanoscale deformation processes within the microstructure of $\sim$1 μm thin films of ePP. Series of SFM images taken during straining and relaxation show a large variety of deformation processes: elongation, bending, kink formation, and fragmentation of individual crystalline lamellae into 10 nm large blocks (M. Franke, R. Magerle, to be published). The setup allows for different mechanical testing schemes, such as step-wise straining with simultaneous measurement of the temporal evolution of stress overshoot and relaxation. The stress relaxation process ranges over several hundreds of seconds and it resembles the stress relaxation behavior observed in polymer melts. Other experiments are straining with a constant straining rate, creep experiments at constant stress, and shearing. From this data viscoelastic material parameters, such as the elastic modulus and the elongational viscosity can be determined.

CPP 23.3 Tue 18:00 P2

Multi-Setpoint Amplitude Modulation Atomic Force Microscopy on Soft Materials — •Eike-Christian Spitzner, Christian Riesch, Mario Zerson, and Robert Magerle — Chemische Physik, TU Chemnitz, D-09107 Chemnitz, Germany

We present an approach where pointwise measurement of amplitude and phase as function of tip sample distance is used to reconstruct amplitude modulation atomic force microscopy (AM-AFM) images. From one single-pass measurement, images for almost any amplitude setpoint are reconstructed. Furthermore, the position of the unperturbed surface, and the tip indentation into soft (compliant) specimens is determined. Tip indentation can be used as a depth coordinate to reconstruct depth-resolved cross-sections and volume images of the mechanical properties of the top 20 nm of soft polymeric specimens. The method overcomes most limitations of AM-AFM and allows for a better and more quantitative interpretation of height and phase images. The materials studied include block copolymer microdomains, crystalline lamella in elastomeric polypropylene, surfaces of poly(3-hexylthiophene), and supramolecular aggregates deposited on a substrate.

CPP 23.4 Tue 18:00 P2

Nucleation and crystallization in polycaprolactone (PCL) — •Andreas Wurm[1], Doris Pospiech[2], and Christoph Schick[1] — [1]University of Rostock, Institute of Physics — [2]Leibniz IPF Dresden e.V.

Crystallization is commonly considered as nucleation followed by a growth process. Nevertheless, a complete description of polymer crystallization is far from being achieved. Here we apply the recently developed technique, differential fast scanning calorimetry (DFSC), for the investigation of polycaprolactone (PCL) of different molecular weights. DFSC allows temperature control of the sample and determination of its heat capacity during temperature treatments at high cooling and heating rates (up to 500,000 K/s). We can derive information about kinetics of crystal nucleation and overall crystallization in the whole temperature region between glass transition and melting temperature.

CPP 23.5 Tue 18:00 P2

Conformational changes of oligo(ethlene glycol) under aqueous conditions during growth and at elevated temperature monitored with PMIRRAS — •Stefan Zorn, Alexander Gerlach, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany

Oligo(ethylene glycol) SAMs are a model system for protein resistant SAMs and are subject of comprehensive research for a better understanding of protein resistance. Recent SFG and IR studies show a strong effect of water on the SAM structure and imply a connection of this interaction to the biofouling properties [1]. The exact mechanism, however, is still under discussion. In this study we were able to monitor the growth of hexa(ethylene glycol) SAMs in real-time under aqueous conditions (in-situ) with polarisation modulation infrared spectroscopy (PMIRRAS) using a home built thin liquid layer cell. Fitting of the absorption modes with Gaussians enabled us to determine their area, width and position. We observed a conformational reordering of the OEG moiety from all-trans / helical to predominantly helical and an enhancing crystallinity. In addition, we were able to study the SAM-water interaction in the different growth states. It is the higher the lower the surface coverage [2]. Further, we investigated hexa(ethylene glycol) SAMs at elevated temperatures under in-situ conditions. Our observations contribute to the understanding of biofouling properties and stability of OEG-SAMs and show the possibilities and importance of PMIRRAS in-situ investigations. [1] M.W.A. Skoda et al., Langmuir 23 (2007) 970; [2] S. Zorn et al., PCCP 12 (2010) 8985

CPP 23.6 Tue 18:00 P2

Increasing the disorder-order transition temperature in PS-P2VP diblock copolymers by applying strong electric fields — •Ilja Gunkel and Thomas Thurn-Albrecht — Institute of Physics, Martin Luther University Halle Wittenberg, Halle, Germany

We present temperature-dependent in-situ small-angle X-Ray scattering measurements on symmetric polystyrene-block-poly-2-vinylpyridine (PS-P2VP) diblock copolymer melts in the presence of an electric field. We found that an electric field favors the ordered state in diblock copolymer melts as the temperature of the disorder-order transition (T_{DOT}) was increased by 1 °C in the presence of electric fields with 30 V/μm. This result qualitatively agrees with recent theoretical predictions on the shift of T_{DOT} in electric fields where it was shown that applying an electric field suppresses composition fluctuations thus leading to an increase of the disorder-order transition temperature [1]. However, in concentrated solutions of symmetric PS-PI in toluene T_{DOT} was found to decrease in the presence of electric fields [2]. These different results will be compared and discussed.

[1] Gunkel, I.; Stepanow, S.; Trimper, S.; Thurn-Albrecht, T. Macromolecules 2007, 40 (6), 2186-2191

[2] Schoberth, H. G.; Schmidt, K.; Schindler, K. A.; Boker, A. Macromolecules 2009, 42 (10), 3433-3436.

CPP 23.7 Tue 18:00 P2

Polymer Blend Lithography: A Method to Generate Monolayer Templates for the Self-Assembled Growth of ZnO Nanostructures — •Jiehong Jin[1], Armin Müller[1], Svetlana Khasminskaya[1], Cheng Huang[1], Jorg Pfeifer[1], Luciana Pitta Bauermann[3,4], Peter Gerstel[3,4], Joachim Bill[3,4], Stefan Walheim[1,2], and Thomas Schimmel[1,2] — [1]Karlsruhe Institute of Technology (KIT), Institute for Nanotechnology (INT), Karlsruhe, Germany — [2]Karlsruhe Institute of Technology (KIT), Institute of Applied Physics and Center for Functional Nanostructures (CFN), Karlsruhe — [3]Institute for Materials Science, Universität Stuttgart, Germany — [4]Max-Planck-Institute for Metals Research, Stuttgart

A wet-chemical process near room temperature allowing the large-area deposition of nanostructured ZnO films would be attractive for device fabrication. Our approach is 1) to generate a monolayer template on which 2) a nanostructured ZnO layer is assembled. Polymer phase separation during spin coating of a polymer blend is used to generate a purely lateral phase morphology. The selective dissolution of one polymer (Polystyrene) leaves back a polymer mask (PMMA) with holes showing sharp edges. The diameter of the holes depends on the humidity, the molecular weight and film thickness and can therefore be adjusted in the range between 100 nm and several microns. We use these perforated polymer films as lift-off masks for the deposition of self-assembled silane monolayers. The remaining 2-nm-thick pattern can be used as template for the wet-chemical assembly of large-area ZnO nanostructures with thickness of about 50 nm.

CPP 23.8 Tue 18:00 P2

Ellipsometry as a non-destructive tool for in-depth analysis of polymer/fullerene blend films — •Sebastian Engmann, Vida Turkovic, Harald Hoppe, and Gerhard Gobsch — Technische Universitaet Ilmenau, Fakultaet fuer Mathematik und Naturwissenschaften, Institut fuer Physik, Experimentalphysik I, Weimarer

Strasse 32, 98693 Ilmenau, Germany

The validity of various optical descriptions/models in relation to the blending ratio of polymer/fullerene blends used in organic photovoltaics has been tested. Fullerene inclusions shape and the degree of polymer crystallinity inside the film have been investigated using Spectral Ellipsometry.

CPP 23.9 Tue 18:00 P2

Self-aggregation of mononucleotides in solution studied by frequency resolved depolarized dynamic light scattering techniques — •Christoph Angermann[1] and Thomas Hellweg[2] — [1]Universität Bayreuth, Physikalische Chemie 1 — [2]Universität Bielefeld, Physikalische und Biophysikalische Chemie

In some cases the rotational diffusion of particles in the nanometer scale is too fast to be easily resolved with conventional photon correlation spectroscopy (PCS) methods. Therefore a custom built depolarized 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. The original setup was enhanced with an AOM (acousto-optic modulator) instead of mechanical shutters. Due to this enhanced measurement technique, it is easily possible to accumulate the noisy component efficiently leading to an enhancement of the signal to noise ratio. As a proof of principle for the experimental technique we studied interesting self-assembly of mononucleotides in aqueous solution. Self-aggregation phenomena as well as the interaction of the mononucleotides uridine-5'-monophosphate and cytidine-5'-monophosphate can be analyzed precisely.

CPP 23.10 Tue 18:00 P2

Direct estimation of spin diffusion constants by a cross-polarization based method — •Matthias Roos and Günter Hempel — Martin-Luther-Universität, Institut für Physik, Betty-Heimann-Straße 7, D-06120 Halle

Spin diffusion often influences the results of relaxation experiments in dependence of structural and dynamic heterogeneities of the sample. Therefore this phenomenon can be used for the estimation of such heterogeneities. Knowledge of the magnitude of the spin diffusion constant is a precondition for those investigations. Theoretical approaches for the estimation of this constant were used sometimes which however particularly in more mobile phases give rise to some uncertainty. Few experimental attempts for estimating this constant are known. Here we introduce a method which makes use of cross polarization between protons and 13C spins. This method produces holes in the proton magnetization at places where 13C spins are neighboured. During the following waiting time the holes are re-filled. This filling process is caused by spin diffusion; its speed contains information about the spin-diffusion constant. We follow the hole filling process by another cross polarization.

Applications to liquid crystals and polymers (amorphous and crystalline regions) are demonstrated. In a liquid crystal (7CB) the diffusion process could be proven as being one-dimensional.

CPP 23.11 Tue 18:00 P2

Self-Assembled Monolayers of Heteroarene Macrocycles — •Stefan-Sven Jester, Eva Sigmund, and Sigurd Höger — Rheinische Friedrich-Wilhelms-Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn

Nanoscale shape-persistent macrocycles based on dithiophene corner units, linked via phenylene-ethynylene-butadiynylene units, are synthesized. Self-assembled monolayers of macrocycles of different ring sizes (n=3-6) are investigated using scanning tunneling microscopy at the solid-liquid-interface.

CPP 23.12 Tue 18:00 P2

Oligomers and Cyclooligomers of Rigid Phenylene-Ethynylene-Butadiynylenes: Synthesis and Self-Assembled Monolayers — •Stefan-Sven Jester, Natalia Shabelina, Stephan M. Le Blanc, and Sigurd Höger — Rheinische Friedrich-Wilhelms-Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn

Starting from the same bisacetylene, different reaction conditions (palladium or copper catalysis) selectively yield cyclic or acyclic oligomers with n=2-6 linked by freely rotating corner units. STM images of self-assembled monolayers reveal the difference in the adsorption behavior of the acyclic and cyclic oligomers.

CPP 23.13 Tue 18:00 P2

Monolayer Patterns for Templated Self-Assembly of ZnO Films with Nanoscale Resolution — •Svetlana Khasminskaya[1], Armin Müller[1], Jiehong Jin[1], Cheng Huang[1], Jorg Pfeifer[1], Luciana Pitta Bauermann[3,4], Peter Gerstel[3,4], Joachim Bill[3,4], Stefan Walheim[1,2], and Thomas Schimmel[1,2] — [1]Karlsruhe Institute of Technology (KIT), Institute for Nanotechnology (INT), Karlsruhe, Germany — [2]Karlsruhe Institute of Technology (KIT), Institute of Applied Physics and Center for Functional Nanostructures (CFN), Karlsruhe — [3]Institute for Materials Science, Universität Stuttgart, Germany — [4]Max-Planck-Institute for Metals Research, Stuttgart

Lithographically defined self-growing ZnO films were prepared by a bioinspired chemical bath deposition technique (CBD). We observed a high selectivity of ZnO deposition: Teflon-like per-fluoro-decyl-trichlorosilane (FDTS) monolayers repelled ZnO primary particles, whereas amino-functionalized areas of the substrate were selectively covered by a highly anisotropic, oriented, and compact ZnO film with a thickness of 50 nm. The size of the primary particles in our methanol-based solution was approximately 2.5 nm. On the amino substrate they formed agglomerates not larger than 30 nm. Monolayer patterns made by polymer blend lithography were templated with an edge resolution of 30 nm.[1].

[1] L. Pitta Bauermann et al.; Langmuir, 2010, 26 (6), pp 3774-3778

CPP 23.14 Tue 18:00 P2

Morphological study of Langmuir films of Polyglutamate — •Renate Reiter[1], Frédéric Wintzenrith[2], and Günter Reiter[1] — [1]Physikalisches Institut, Universität Freiburg, Germany — [2]Ecole Polytechnique, France

Langmuir monolayers are ideal systems for experimental studies of two dimensional physical phenomena. Poly-γ-benzyl-L-glutamate (PBLG) forms rigid rods with flexible side chains when it is in α-helical conformation. Liquid crystalline- and gel-phases have been observed in organic solvents. When these hydrophobic molecules are confined to the air water interface, the rods lay down flat and can form network-like structures. We want to understand the mechanisms governing the formation of these structures. With a Langmuir trough we investigated phase transitions in such PBLG- layers by recording surface pressure (π) versus area (A) isotherms. Furthermore, the temporal evaluation of π gave valuable information on relaxation processes. The obtained film morphologies were visualized directly on the water surface by means of BAM and, after film transfer onto solid substrates, with AFM. Our results strongly suggest that isotherms recorded in the standard way do never represent equilibrated states. At constant area, a complex, non-uniform decay of π in time was observed indicating molecular rearrangement. At high packing densities π slowly decays to zero. Surprisingly, even after such relaxation, a layer with fibrillar morphology was transferred. Moreover, the isotherms showed intricate hysteretic and relaxation behavior. Can we achieve nematic-like structures in quasi 2D films?

CPP 23.15 Tue 18:00 P2

Einflüsse von Polymeren auf die Kollagenassemblierung — •Nora Haufe[1], Doreen Naumburger[1], Sébastien Garnier[2], Günter Scherr[2], Volker Bach[2] und Michael Mertig[1] — [1]Professur für Physikalische Chemie, Mess- und Sensortechnik, TU Dresden, 01062 Dresden — [2]BASF SE, 67063 Ludwigshafen

Kollagen ist die wichtigste strukturgebende Komponente der Haut. Daher wird bovines Typ I Kollagen als Modell erforscht, um die Gerbung besser zu verstehen.

Die *in vitro* Assemblierung ist eine Untersuchungsmethode, die Informationen auf molekularer Ebene sowie höheren Struktureinheiten zuläßt. Sie gibt Aufschluss über Wechselwirkungen von Monomeren bishin zu Fibrillen und stellt daher ein geeignetes Betrachtungssystem dar.

Polymere beeinflussen diesen Prozess. Polyethylenglycol und Polyacrysläure als zwei nichtgerbende Polymere und die nachgerbende Polymethacrylsäure wurden vergleichend zum kovalent bindenden Glutaraldehyd untersucht.

Spektroskopische und mikroskopische Untersuchungen werden parallel genutzt, um Rückschlüsse auf Wechselwirkungen in den verschiedenen hierarchischen Niveaus zu ziehen. Veränderungen der Assemblierungskinetik können in Abhängigkeit von Menge und Art des Polymers durch Trübungsmessungen detektiert werden. Mittels Rasterkraftmikroskopie werden morphologische Unterschiede der gebildeten Fibrillen untersucht.

CPP 23.16 Tue 18:00 P2

Behaviour and Assembly of Janus Particles in Confined Systems — •Julie Murison and Matthias Schröter — Max Planck Insitute of Dynamics and Self Organization, Göttingen

Half hydrophobic Janus Particles were created using a pickering-style emulsion. The degree of Hydrophobicity was controlled using different surfactants to create a portfolio of beads. Self Assembly of these particles at the air/water and oil/water interfaces was studied using X-ray Tomography. Beads are found to form micelle like structures within the bulk and create distinct regions of wettability. The packings are useful to model natural porous systems of heterogeneous wettability such as petroleum reservoirs.

CPP 23.17 Tue 18:00 P2

Supramolecular Self-Assembly of Hydrogen Bonded Bis-Urea Based Molecules — •Roozbeh Shokri[1,2], Ashok Narladkar[2], Laurent Simon[2], Fraçois Vonau[2], Laurent Bouteiller[3], and Günter Reiter[1,4] — [1]Physikalisches Institut, Universität Freiburg, Hermann-Herder-Strasse 3, 79104 Freiburg, Germany — [2]Institut de Science des Matériaux de Mulhouse (IS2M-LRC7228), 4 rue des Frères Lumière, 68093 Mulhouse, France — [3]Laboratoire de Chimie des Polymères, UMRb7610, Université Pierre et Marie Curie, 4 place Jussieu, 75252 paris CEDEX 05, France — [4]Freiburg Institute for Advanced Studies (FRIAS), 79104, Freiburg, Germany

The process of self-assembly has been investigated by AFM analysis for three different bis-urea substituted toluene molecules, EHUT, 3EOUUT and C12EHUT with different side chains. Indirect measurements (neutron-scattering,...) and calculations led to conclude that in solution EHUT molecules can form long supramolecular nanotubes at specific conditions of temperature and concentration. Here, we studied the possibility to stabilize these nanotubes on a surface and see them directly by AFM. Our study, however, presents evidences for layered structures on mica with a quantized step-height of around 2 nm. We prove that within these layers the molecules are organized in a unique upward conformation and form ribbons through hydrogen bonding. Molecules with different side-groups, 3EOUUT and C12EHUT showed characteristic lamellar and triangular morphologies when deposited on graphite, reflecting the 3-fold anisotropy of the atomic lattice of graphite. The second layer in registry with the first layer was observed.

CPP 24: Poster: Polymer Dynamics

Time: Tuesday 18:00–20:00 Location: P2

CPP 24.1 Tue 18:00 P2

Adsorption and external stimulation of single polymer chains — •Kirsten Dammertz, Alexander Gerstmayr, Masoud Amirkhani, and Othmar Marti — Department of Experimental Physics, Ulm University

In the presented work, we study the behavior of externally stimulated single polymer chains (exposed to different vapors or electric fields) interacting with substrates like mica or graphite. Conformational changes and reorientation of adsorbed polymers are visualized by means of an advanced, custom-made atomic force microscope (AFM).

To verify our data and analyze the underlying chemical and physical processes, we perform molecular dynamics (MD) simulations. Moreover, we use Monte Carlo (MC) and density functional theory (DFT) simulation techniques to improve our analysis and to compare the experimental result with prior assumptions [1,2].

[1] Gallyamov et al., Macromol. Rapid Commun. 2005, 26, 456-460

[2] Gallyamov et al., Macromol. Chem. Phys. 2007, 208, 164-174

CPP 24.2 Tue 18:00 P2

Monte Carlo Studies of Semiflexible Branched Polymers — •Ganna Berezovska, Maxim Dolgushev, and Alexander Blumen — Hermann-Herder-Straße 3, D-79104 Freiburg, Germany

An important class of macromolecules are the branched polymers. Their properties depend both on their topology (in which the branching points play a fundamental role) and also on the degree of semiflexibility of their segments. While analytical investigations are possible under idealized conditions [1], numerical simulations are required under more realistic situations. Here we make use of the bond fluctuation model (BFM). While previous investigations used BFM ideas either for flexible branched structures or for semiflexible linear chains, our simulations allow to account both for branching and also for semiflexible behavior. Examplary, we apply the method to study polymers, whose topological structures correspond to the simplest pair of cospectral graphs. Such graphs are mathematically and chemically very important since they have the same Laplacian spectra although being topologically different. Hence, in a generalized Gaussian framework, flexible polymers whose structures are cospectral graphs are predicted to be indistinguishable under usual dynamical measurements. According to our new mathematical-analytical study [2], introducing semiflexibility allows to differentiate between such pairs of polymers. This is qualitatively confirmed by our simulation results [2].

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

[2] M. Dolgushev, G. Berezovska, A. Blumen, J. Chem. Phys. 133, 154905 (2010).

CPP 24.3 Tue 18:00 P2

Segregation of Identical Flexible Chains in Solution — •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 study the segregation of two long chains from parallel but randomly twisted start conformations under good solvent conditions using Monte Carlo simulations. For investigation of the segregation process we focus on the center of mass separation between the two chains and the average square distance between the monomers which were connected before segregation starts. We argue that segregation is dominated by free diffusion of the chains assuming that untwisting can be achieved by Rouse-like fluctuations on the length scale of the twisted loop. The free diffusion hypothesis is confirmed in the scaling analysis of individual chain dynamics, and segregation measures follow this scaling nearly. Long chains, however, show retardation effects which can be described by a new dynamical exponent which is slightly larger than the dynamical exponent for Rouse-like diffusion. Our results indicate that nearly free diffusion of chains during a time scale of a few Rouse-times can lead to segregation of chains. These results are applicable for DNA in eukaryotic cells and their chromatin segregation after replication.

CPP 24.4 Tue 18:00 P2

Multiple-quantum NMR observations of constraint release and contour-length fluctuation — •Marie-Luise Lehnich and Kay Saalwächter — Institut für Physik-NMR, Universität Halle, Betty-Heimann-Str. 7, 06120 Halle

The behaviour of entangled melts is still not fully understood. The predictions of de Gennes' famous reptation concept can be observed directly with ^{1}H multiple-quantum NMR. We monitor the dynamics of long-chain polymer melts over 5 decades in time. The regimes II-IV of the tube model are covered with this technique. The fixed-tube model, which is a combination of Rouse theory for unentangled melts and the reptation model, describes the mechanical data insufficiently. This causes ongoing discussions on also including the dynamics of the tube itself. Contour-length fluctuations (CLF) and constrained release (CR) could be the reason for the motion of the tube.

In extending previous work [1], we diluted protonated chains in matrices of deuterated chains, which are invisible in ^{1}H NMR. With this method, the influence of the "tube" can be analysed in an isolated fashion. The effects of CR and CLF can be separately studied.

[1] F. Vaca Cháves and K. Saalwächter. NMR Observation of Entangled Polymer Dynamics: Tube Model Predictions and Constrained Release, Phys. Rev. Lett., 104, 198305 (2010)

CPP 24.5 Tue 18:00 P2

Zipping dynamics of semiflexible polymers — Fabian Heisterkamp and •Jan Kierfeld — Technische Universität Dortmund, Fakultät Physik, Otto-Hahn-Str. 4, 44227 Dortmund, Germany

The adhesion or zipping of two polymers plays an important role in many biological processes, for example the formation of filament bundles in the cytoskeleton. We investigate the dynamics of a zipping process with polymer ends attached to two large beads using Brownian dynamics simulations and analytical arguments. In the limit of large adhesion we find circular trajectories of the end beads. Simulations for realistic parameter values exhibit deviations due to bending forces and buckling.

CPP 24.6 Tue 18:00 P2

Rotational and translational diffusion in hyperbranched polyglycerols — •Tilman Schubert, Joshua Rume Sangoro, Ciprian Iacob, and Friedrich Kremer — Institute of Experimental Physics I, University of Leipzig, Linnéstr. 5, 04103 Leipzig, Germany

Molecular dynamics of hyperbranched polyglycerols of different molecular weights is studied by Broadband Dielectric Spectroscopy (BDS). The results for the characteristic quantities (structural alpha-relaxation rate and diffusion rate) are combined with the findings of PFG-NMR, rheology and calorimetry. Three different dielectric relaxation processes are observed. Upon application of Maxwell's relation to the rheology data structural relaxation rates are obtained corresponding to the slowest dipolar relaxation from BDS measurements. Extrapolated to lower temperatures, agreement is found with the glass transition temperatures measured by DS calorimetry. The results are discussed within the framework of recent theories of the dynamic glass transition.

CPP 24.7 Tue 18:00 P2

Patterned Polymer Carpets — •Ihsan Amin[1], André Beyer[2], Marin Steenackers[3], Rene Schubel[1], Ning Zhang[3], Armin Gölzhäuser[2], and Rainer Jordan[1] — [1]Professur für Makromolekulare Chemie, Department Chemie, TU Dresden, Zellescher Weg 19, 01069 Dresden, Germany — [2]Physik supramolekularer Systeme, Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany — [3]Wacker-Lehrstuhl für Makromolekulare Chemie, TU München, Lichtenbergstrasse 4, 85747 Garching, Germany

We report on the first example for the fabrication of patterned polymer carpets. Polymer brushes of styrene and 4-vinyl pyridine were grafted by self-initiated surface photopolymerization and photografting (SIPGP) on a 2D framework of fully crosslinked and chemically patterned nanosheets. The grafted polymer brushes were observed over the entire nanosheets with a preferred grafting on the functionalized nanosheet areas. This results in continuous polymer carpets with an intact nanosheet framework but with amplification of the chemical patterning into a 3D topography of the grafted polymer brush. In the case of negative patterned nanosheet, the patterned carpet could be prepared as freestanding ultrathin membranes. Furthermore, swelling experiments with poly(4-vinyl pyridine) carpets showed that the direction of the resulting buckling of the flexible carpet is correlated to the patterning. This may open the possibility of the development of micro- or nanoactuator devices with anisotropic responds upon environmental changes.

CPP 25: Colloids and Complex Liquids I - Structure

Time: Wednesday 10:30–13:00 Location: ZEU 222

Topical Talk CPP 25.1 Wed 10:30 ZEU 222

From elementary building blocks towards colloidal molecules — Claudia Simone Wagner and •Alexander Wittemann — Physikalische Chemie I, Universität Bayreuth, Universitätsstr. 30, 95440 Bayreuth, Germany.

We report on the fabrication of clusters and binary colloidal composites made from organic and inorganic nanoparticles. Control over the assembly of nanoscale functional building units is of great significance to practical applications, but is also interesting from a more fundamental point of view of understanding the self-assembly of nanostructured materials. Joining together different spherical nanoparticles in a defined manner allows control over the shape, composition and surface roughness of the nanocomposites. If the constituents consist of different materials, the resulting heteroaggregates feature both compositional and interfacial anisotropy, offering unprecedented perspectives for rationally designed functional colloids, which are of fundamental importance to a broad range of applications including sensing, photonic, and electronic devices. The preparation of the clusters is based on the agglomeration of particles that are dispersed in an emulsion. The droplet size distribution in the emulsion is controlled by ultrasound. The particles adsorb on the surface of the emulsion droplets (Pickering effect) and coagulate in a well-defined way during the evaporation of the (dispersed) oil phase. Using this method one can produce clusters with colloidal dimensions (<400nm). We will report on the shapes and yield of these clusters using electron microscopy, scattering methods, and differential centrifugal sedimentation.

CPP 25.2 Wed 11:00 ZEU 222

Computer simulations of cluster formation via emulsion droplet evaporation — •Andrea Fortini, Ingmar Schwarz, and Matthias Schmidt — Theoretische Physik II, Physikalisches Institut, Universität Bayreuth, D-95440 Bayreuth, Germany

Using kinetic Monte Carlo simulations, we investigate a theoretical model of colloidal particles that interact with short-ranged attraction and long-ranged repulsion. A second hard-sphere component represents emulsion droplets that interact only with an attractive well with the colloids. The potential well has a minimum at the droplet surface and induces the Pickering effect. The droplets are taken to shrink in time, in order to model experimental conditions of droplet evaporation. We investigate the resulting morphology of colloidal clusters that have formed after complete evaporation of the droplets. We find stable packings that range from sphere doublets, triangles, and tetrahedra to complex polyhedra. We compare the resulting structures with experimental results [1,2].

[1] Manoharan et al. Science (2003) 301, 483.
[2] Wagner et al. Langmuir (2008) 24, 12126.

CPP 25.3 Wed 11:15 ZEU 222

Pattern formation of colloidal suspensions by dip-coating: An in-situ grazing incidence X-ray scattering study — •Jan Perlich[1], Matthias Schwartzkopf[1], Volker Körstgens[2], Peter Müller-Buschbaum[2], Rainer Gehrke[1], and Stephan V. Roth[1] — [1]HASYLAB-DESY, Notkestr. 85, D-22603 Hamburg (Germany) — [2]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, D-85748 Garching (Germany)

The dip-coating technique is one of the commonly applied methods for the preparation of thin films or the patterning of templates from polymer solutions and particle suspensions. We present an in-situ investigation of the dip-coating process of colloidal suspensions by the advanced scattering technique grazing incidence small angle X-ray scattering (GISAXS). The focus is on the real-time monitoring of the vertical dip-coating process to deliver an insight of the structural changes during pattern formation. With the selected measurement configuration a fixed spot on the sample surface is probed and the structural information at the time the contact line passes through the beam-illuminated area is obtained, hence revealing the structure at the vicinity of the flowing meniscus. After the in-situ GISAXS experiments, the as-prepared samples are analyzed by optical microscopy (OM) for an overall homogeneity check of the dip-coated thin film. Finally, the surface structures are investigated by atomic force microscopy (AFM), yielding topographic images and thus real space information about the structure heights and widths.

CPP 25.4 Wed 11:30 ZEU 222

Crystallization and vitrification of a hard sphere like colloidal model system — Markus Franke and •Hans Joachim Schöpe — Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz

A complete understanding of the solidification process is one of the long standing problems in condensed matter physics. The use of colloidal model systems provides an ideal controlled experimental system to reduce this lack of knowledge. We investigated the solidification scenario in suspensions of gravity matched colloidal hard spheres (HS) using time resolved static light scattering as well as dynamic light scattering techniques. A detailed analysis of crystal nucleation path ways shows that crystallization is originated by transient precursors (structurally heterogeneous clusters; structural heterogeneities) during the induction stage. Later these convert into highly ordered crystals in a fast, activated process. Following the same processes over a range of volume fractions from near freezing, to above the glass transition allows to systematically link the mechanisms involved in HS crystallization to those of the HS glass transition.

CPP 25.5 Wed 11:45 ZEU 222

Binary mixture of charged colloidal spheres with a spindle-type phase diagram — •Janina Marquis, Nina Lorenz, and Thomas Palberg — Institute of Physics, University of Mainz, Germany

Colloidal suspensions are an important model system for solid state physics and statistical mechanics. Their phase behaviour and crystallization kinetics are conveniently accessible via optical methods like light scattering and microscopy.

We have studied the phase behaviour and other properties of a deionized binary mixture of charged colloidal spheres with a size ratio of $\Gamma = \frac{a_s}{a_l} = 0.90$ and a charge ratio of $\Lambda = \frac{Z_s}{Z_l} = 0.8$ as a function of composition. Here the screened Coulomb interaction is increased by increasing the total particle number density (sulphate stabilized Polystyrene-Poly-n-Butylacrylamide copolymer particles: diameter: $2a_s = 118$nm, $2a_l = 131$nm, effective charges from elasticity: $Z_s^{\mathrm{eff}} = 401 \pm 20$, $Z_l^{\mathrm{eff}} = 499 \pm 21$). Both pure samples and the mixtures crystallize in a bcc structure with the latter forming random substitutional crystals. The liquidus as a function of composition stays roughly horizontal, whereas the solidus curves symmetrical to higher number densities and the coexistence region is widened to a horizontally oriented spindle. Similarities and differences to other charged sphere mixtures are discussed [1, 2].

[1] N. J. Lorenz et al.: J. Phys.: Condens. Matter 21, 464116 (2009)
[2] N. J. Lorenz, T. Palberg,: J. Chem. Phys. 133 104501 (2010)

CPP 25.6 Wed 12:00 ZEU 222

Modification of critical adsorption profiles by addition of ions — •Julian Dietrich[1], Ursula Nellen[1], and Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [2]Max-Planck-Institut für Metallforschung, Heisenbergstraße 3, 70569 Stuttgart, Germany

In the last years there is growing interest in the use of binary liquids as dispersion medium for colloidal systems because this leads e.g. to critical Casimir forces or the formation of bicontinuous gels (bijels). We investigate the role of additional salt ions in binary mixtures close to the critical point since this may lead to interesting coupling effects between electrostatic forces and the mixtures' concentration distribution. In our experiments we study the adsorption profile of a critical water/2,6-lutidine mixture in the presence of salt ions. Such temperature-dependent profiles are obtained by measuring the variation of the permittivity with a surface plasmon resonance experiment for different types and concentrations of salts. We compare these results to chemically modified surfaces where the adsorption preference for one of the mixture's components is systematically altered.

CPP 25.7 Wed 12:15 ZEU 222

Excluded Volume Effects in the Depletion Attraction between Nanoparticles — •Maryam Naderian[1,2], Matthias Fuchs[2], and Michel Rawiso[3] — [1]Institut für Elektrochemie, Universität Ulm, Germany — [2]Universität Konstanz, Germany — [3]Institut Charles Sadron, Strasbourg, France

We study the correlation functions and the interparticle interactions of mixtures of nonadsorbing real polymers and colloidal particles in both nanoparticle and colloid limits employing extensive numerical calculations within the framework of an integral equation method (PRISM) [1]. In our theoretical model colloidal particles considered as hard spheres and polymers are described using a form factor from Edwards-Flory mean field theory capturing self avoiding walk correlations.

Keeping the colloidal particle volume fraction low and varying the polymer concentration from infinitely dilute to semidilute we investigated the effect of the excluded volume interaction between the polymer monomers on the depletion layer and the induced interaction between the particles. Using numerical solutions of the PRISM-mPY equations the thermodynamic consistency is achieved, the radial distribution functions and second virial coefficient among the colloidal particles are investigated. At the end our theoretical predictions are compared with the existing results from the field theoretical approach [2] and the experimental data.

[1] K.S. Schweizer and J.G. Curro. Adv. Polym. Sci., 116:319, 1994.

[2] E. Eisenriegler. Field Theory of polymer Interactions. WILEY-VCH Verlag Berlin GmbH, 2005.

CPP 25.8 Wed 12:30 ZEU 222

Is there a hexatic phase in quasi-2d? — •Nadezhda Gribova, Axel Arnold, and Christian Holm — ICP, Universität Stuttgart, Stuttgart, Germany

A quasi-2d system, a 3d system that is constrained in one of the directions, is expected to combine some characteristic properties both of 2d systems and of 3d systems. One of the most interesting features of 2d systems is the existence of a hexatic phase, an intermediate phase in the liquid-to-solid transition.

The presence of this transition in quasi-2d systems is an open question, and even in 2d systems it is still under discussion. In our work we report a computer simulation study of a Lennard-Jones liquid confined in a narrow slit pore with tunable attractive walls. In order to investigate how the freezing in this system occurs, we perform an analysis using a broad range of order parameters that have been used so far to investigate the existence of the hexatic phase in 2d systems. It turns out, that although some of the parameters indicate that the system goes through a hexatic phase, other parameters exclude it. This shows that to be certain whether a system has a hexatic phase, one needs to study not only a big system, but also several order parameters to check all necessary properties. We observe an intermediate hexatic phase only in the slit with extremely attractive walls and a single layer of particles, i. e. if the system is practically perfectly 2d.

CPP 25.9 Wed 12:45 ZEU 222

Computing absolute free energies of 2d colloidal crystals under confinement — •Dorothea Wilms, Peter Virnau, and Kurt Binder — Johannes Gutenberg Universität, Mainz

A two-dimensional colloidal crystal is studied under the confinement of structured and planar 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 as the left-over particles (which no longer fit into the crystalline structure if one row disappears) have to distribute themselves in the crystal.

A strong hysteresis is observed at this transition if only the stress is computed. Therefore, we have applied a recently developed method to compute absolute free energies of disordered structures in order to investigate this transition in more detail. Thus we were able to determine the transition point with much higher precision. We have also used the same method in order to compute the interfacial tension of the crystal with the walls.

CPP 26: Polymer Dynamics

Time: Wednesday 10:30–11:45 Location: ZEU 160

CPP 26.1 Wed 10:30 ZEU 160

Local mobilities and chain end effects in non-entangled polymer melts - a molecular dynamics simulation study — •Diddo Diddens[1,2] and Andreas Heuer[1,2] — [1]Institut für physikalische Chemie, Universität Münster, Corrensstraße 30, 48149 Münster, Germany — [2]NRW Graduate School of Chemistry, Corrensstraße 36, 48149 Münster, Germany

The dynamics of a polymer chain in a dense, non-entangled melt can be well described by the Rouse model. Within this model, the chain is composed of a series of Brownian beads connected by harmonic springs, where each bead is characterized by a uniform friction coefficient imposed by the surrounding chains. However, when probing the bead's mean square displacement, the chain ends move faster than the central monomers for topological reasons, and the chain ends have on average more intermolecular neighbors.

Using a newly developed method [1] we study the dependence of the local chain dynamics on the bead position by direct determination of the local friction coefficient. In this way, the Rouse assumption of uniform friction coefficients along the entire chain and specifically at the chain end is tested for an all-atom MD simulation of a poly(ethylene oxide) (PEO) melt. In particular, the interplay of the surroundings of a given monomer and the friction coefficient is discussed. Furthermore we analyze whether the forward-backwards dynamics of the monomers is compatible with the predictions of the Rouse model.

[1] D. Diddens, M. Brodeck, A. Heuer, EPL 91 (2010) 66005

CPP 26.2 Wed 10:45 ZEU 160

Short time dynamics of medium length molecules — •Humphrey Morhenn[1], Sebastian Busch[1], Dieter Richter[2], and Tobias Unruh[3] — [1]Technische Universität München, Forschungs-Neutronenquelle Heinz Maier-Leibnitz and Physik Department E13, 85747 Garching, Germany — [2]Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [3]Lehrstuhl für Kristallographie und Strukturphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

The description of transport mechanisms in molecular liquids is a challenging task. Especially the mechanism of molecular self-diffusion in liquids of organic medium-chain molecules is not fully understood yet. TOF-QENS experiments were performed on a polyethylene melt (n-$C_{100}H_{202}$), and a polydimethylsiloxane melt (PDMS, molecular weight approx. 17,250). Both chains are long enough to show gaussian chain statistics in their confirmations so that it was possible to check the validity of the Rouse model on this time and length scale. It could be shown that the simple Rouse model cannot describe the TOF-QENS data satisfactorily but respecting a reduced local chain flexibility by a mode dependent friction coefficient the Rouse model can surprisingly reproduce the experimental data of PE down to $t = 1$ ps.

CPP 26.3 Wed 11:00 ZEU 160

Coarse-grained modelling of the spreading of droplets on reactive substrates — •Murat Mulayim and Marcus Muller — Institut für Theoretische Physik, Georg-August-Universität, Göttingen, Germany

We study, by molecular simulation, the statics and dynamics of chemically driven running polymer droplets. The polymer melt is composed of 10-bead chains and described with coarse-grained potentials that retains the main properties of the chains. The substrate is modelled by two layers of a FCC lattice, having density $\rho_s = 2\sigma^{-3}$. The temperature was held constant with a Dissipative Particle Dynamics thermostat that locally conserves momentum and thus leads to hydrodynamic behaviour on long time and length scales. A self-produced wettability is gradient generated under the droplet via changing the type of substrate atoms depending on their spatial position and with a pre-defined probability. Parameters (reaction rate) for observing running polymer droplets in MD simulations are identified and the velocity profile and dissipation mechanisms in the quasi steady-state is presented.

CPP 26.4 Wed 11:15 ZEU 160

Temperature dependent single molecule rotational dynamics in PMA — •subhasis adhikari, markus selmke, and frank cichos — Molecular Nanophotonics Group,Inst. of Expt. Phys. I, Univ. of Leipzig, 04103,Leipzig,Germany

Temperature dependent measurements of the rotational diffusion of single dye molecules in the polymer poly(methyl acrylate) (PMA) are presented and compared to shear viscosity data and numerical simulations of the rotational diffusion process. It is found that single molecule rotational diffusion very accurately follows the Debye-Stokes-Einstein predictions for the shear viscosity without any additional parameter. We employ a simple model of dynamic changes of the rotational speed of a single molecule. This dynamic heterogeneity model is based on a Gaussian distribution of activation energies in a VFTH (Vogel-Fulcher-Tammann-Hesse) type temperature dependence of the polymer viscosity. The simulations explain all experimental details concerning the stretched exponential single molecule relaxation dynamics and the related distributions. They also reveal that the observed distributions are related to the intrinsic physical properties of the polymer but do in general not reflect the instantaneous spread of local viscous properties.

CPP 26.5 Wed 11:30 ZEU 160

Polymer dynamics under uniaxial mechanical stress — Ute Böhme and •Ulrich Scheler — Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden

The influence of uniaxial mechanical stress on the dynamics in semicrystalline polymers has been studied using low-field NMR. While in elastomers a monotonic change of the polymer dynamics, a time-dependent behaviour is found for semicrystalline materials. Under mechanical stress there is creep of the polymer chains, which results in a rearrangement of the crystallites. Though not change in the degree of crystallinity has been found, DSC shows better quality of the crystallites, which is a clear indication of rearrangement of the polymer chains. Low-field NMR using permanent magnets in a Halbach arrangement permit in-situ NMR experiments during stretching. The example of poly(propylene) shows an initial shortening of the transverse relaxation time, which is followed by a prolongation. In a stress-relaxation experiment the stress required to keep a constant elongation decreases exponentially. The transverse relaxation time returns to its initial value with a comparable time constant.

CPP 27: Polymer Self Assembly

Time: Wednesday 12:00–13:00 Location: ZEU 160

CPP 27.1 Wed 12:00 ZEU 160

Piezoelectric Properties of Non-Polar Block Copolymers — •Christian W. Pester[1], Markus Ruppel[1,2], Heiko G. Schoberth[1], Volker S. Urban[2], 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

We elaborate on the effects of electric fields on the domain spacings of poly(styrene-*b*-isoprene) block copolymer nanostructures. Synchrotron Small Angle X-Ray Scattering (SAXS) at the ESRF in Grenoble, France helped us to quantitatively evaluate the interaction between an applied external electric field and domain spacings and allowed the first description of piezoelectric properties in non-polar, non-crystalline soft matter systems, as the domains of both the phase separated and the disordered state react linearly to the strength of the electric field. The distortion is instantaneous, fully reversible and its magnitude compares to other piezoelectric systems. We further study the temperature dependence of this electroactive property and its anisotropic behavior for different chain orientations, which further allowed us important insights into the molecular origin of electric field ↔ polymer chain interactions and the polymer's phase behavior on a microscopic level.

CPP 27.2 Wed 12:15 ZEU 160

Simulation of the co-continuous mesophases in mixtures of triblock copolymers and polymers — •Alexei Karatchentsev and Jens-Uwe Sommer — Leibniz-Institut fuer Polymerforschung, 01069 Dresden, Germany

We model a linear ABA triblock copolymer as a chain of three soft spheres with fluctuating radii of gyration and the distances between their centers of mass [1], [2]. The probability distribution functions for all these quantities that describe a state of the whole molecule were derived in the previous work [1] within the underlying Gaussian chain model. The kinetics of the mesophase separation is driven by a Monte-Carlo algorithm. We simulate the gyroid phase in pure triblock copolymer melts and study in detail its region of stability. Then, we show that adding polymer molecules modeled as soft spheres can stabilize the gyroid structure in triblock copolymer melts and increase its region of stability over that in the pure triblock copolymer systems.

[1] F. Eurich, A. Karatchentsev, J. Baschnagel, W. Dieterich, and P. Maass, J. Chem. Phys. 127, 134905 (2007)

[2] A. Karatchentsev and J.-U. Sommer, "Simulations of the gyroid phase in diblock copolymers with the Gaussian Disphere Model", ac-

cepted in J. Chem. Phys.

CPP 27.3 Wed 12:30 ZEU 160

One-dimensional coordination polymers: towards molecular wires — •Inshad Jumh[1], Mohammed S. Alam[1], Viatcheslav Dremov[1], Nina Fischer[2], Nicolai Burzlaff[2], and Paul Müller[1] — [1]Department of Physics & Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Germany. — [2]Department of Chemistry and Pharmacy & Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Germany.

Wiring on an atomic scale is one of the main goals of modern nanoelectronics. In this context, we studied one-dimensional coordination polymers on insulating surfaces using frequency-modulation atomic force microscopy (FM-AFM). We have deposited a Zn(II) coordination polymer onto mica and silicon oxide surfaces and have observed a significant effect of the surface on the organization of the polymer. On silicon oxide surfaces, linear single polymer strands as well as double helical structures were observed. On mica, however, 2-dimensional networks of intersecting polymer strands were formed. In addition, we have characterized Cu(II) coordination polymers on mica surfaces. However, we could not map a single polymer strands. Instead, we were able to acquire high resolution images of various, more complex patterns. In conclusion, FM-AFM proved to be an effective technique for investigating and classifying potential nanowires under ambient conditions.

CPP 27.4 Wed 12:45 ZEU 160

Superstructuring of bicontinuous foam-like titania nanostructures in thin films — •Martin A. Niedermeier, Florian Schaff, Volker Körstgens, and Peter Müller-Buschbaum — TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany

Thin films of nanostructured titania have received a lot of attention in various applications, e.g. photovoltaics. The beneficial influence of superstructures has been successfully demonstrated in the past [1]. A light trapping effect can lead to enhanced absorption in the film which is a highly desirable property for optoelectronical devices. In our approach, thin titania films are prepared via a sol-gel route leading to a well defined bicontinuous foam-like nanostructure which exhibits a high surface to volume ratio. Using cost-efficient printing techniques the superstructure is applied to the polymer/titania composite film using a master. Finally, calcination in ambient air is used to transfer the titania into its anatase phase. The super- and nanostructure of the films are characterized using several imaging techniques like SEM or AFM as well as GISAXS. The crystallinity and the thickness of the films were analysed with XRD and XRR. UV/Vis measurements were conducted to investigate the superstructure's influence on the optical properties of the film. [1] M. Niggeman, et al., Thin Solid Films, 451-452 (2004) 619-623

CPP 28: Biopolymers and Biomaterials II (jointly with BP)

Time: Wednesday 10:15–13:00 Location: ZEU 260

Invited Talk CPP 28.1 Wed 10:15 ZEU 260

Stretching Proteins out of equilibrium: how extracellular matrix proteins serve as mechanotransducers — •Viola Vogel — Department of Materials, ETH Zürich, Switzerland

While physical factors and material properties regulate many cell functions, the underpinning mechanisms how cells and tissues sense mechanical stimuli and convert them into biochemical signals are not well understood. As cells explore their environments, they pull on extracellular matrix and thereby stretch those proteins that physically connect the exterior microenvironment with the contractile cytoskeleton. Detailed mechanisms will be discussed how the stretching of proteins can switch their functional display. Deciphering how proteins can serve as mechano-chemical signaling switches is not only essential to learn how cells probe and respond to their environments, but it has also far reaching implications in tissue engineering, systems biology and medicine.

CPP 28.2 Wed 10:45 ZEU 260

Formation and Confinement of Actin Networks in Microchambers — •Siddharth Deshpande[1], Dagmar Steinhauser[2], and Thomas Pfohl[1,2] — [1]Chemistry Department, University of Basel, Switzerland — [2]Max Plank Institute for Dynamics and Self Organization, Göttingen, Germany

Our aim is to study the spatiotemporal evolution of biopolymer networks (e.g. actin, collagen, fibrin) with the aid of microfluidics and using a bottom-up approach. We have designed microfluidic devices consisting of microchambers of different shapes and sizes connected to the main channel by narrow connecting channels. High flow conditions can be achieved in the main channel to control the concentration and composition of the aqueous solution while the transport of molecules into the microchambers is governed by diffusion.

Rhodamine labeled actin monomers are used for the experiments and visualized by fluorescence microscopy. Once polymerized, the actin filaments formed inside the chamber are confined and form an entangled actin network, which can be analyzed for various network properties such as connectivity distribution of nodes, length distribution of links, node fluctuations, link fluctuations and fluctuations in the mesh size.

The experiments with actin bundles in confinement show that the persistence length of actin bundles (L_p) increases proportionally with the number of filaments present in a bundle (n) as: $L_p \approx n^{1.3}$. In the next step, we try to form more complex networks using cross-linking proteins such as α-actinin, filamin, HMM and use FRET microscopy to analyze it.

CPP 28.3 Wed 11:00 ZEU 260

Mechanics and Dynamics of Individual Intermediate Filaments — •Bernd Nöding, Susanne Bauch, and Sarah Köster — Courant Research Centre Nano-Spectroscopy and X-Ray Imaging, University of Göttingen, Germany

The mechanical rigidity of a polymer is characterized by its persistence length L_P. In the case of the intermediate filament (IF) protein vimentin, L_P was found to be on the order of one micrometer using static measurement methods. In contrast, we perform dynamic measurements on fluorescently labeled IFs confined in microchannels, thereby realizing the Odijk confinement regime. Since IFs can be classified as semiflexible polymers ($L \approx L_P$) we assume the worm-like chain model for our fluctuation analysis. The channel walls are included as a parabolic potential in our calculations. Interaction of the filament and the confining microchannel gives rise to an additional length scale, the deflection length λ. We combine IF data with literature data for actin. Thereby we can access both the channel dimension d and L_P, which define the scaling law connecting λ and L_P, $\lambda = a \cdot d^{2/3} \cdot L_P^{1/3}$. The scaling law is fully confirmed by our experiments. Additionally our dynamic measurements yield L_P on the order of one micrometer for vimentin filaments.

CPP 28.4 Wed 11:15 ZEU 260

A constitutive law for cross-linked actin networks by homogenization techniques — Denis Caillerie[1], •Karin John[2], Chaouqi Misbah[2], Philippe Peyla[2], and Annie Raoult[3] — [1]L3S-R, BP 53 - 38041 Grenoble Cedex 9, France — [2]LSP, UJF Grenoble & CNRS, BP 87 - 38402 Saint-Martin-d'Hères, France — [3]LMAP5, Université Paris Descartes, 45 rue des Saints Pères, 75270 Paris Cedex 06, France

Inspired by experiments on the actin driven propulsion of micrometer sized beads we develop and study a minimal mechanical model of a two-dimensional network of stiff elastic filaments grown from the surface of a solid circle. Starting out from a discrete model of the network structure and of its microscopic mechanical behavior we derive a macroscopic constitutive law by homogenization techniques. We calculate the axisymmetric equilibrium state and study its linear stability depending on the microscopic mechanical properties. We find that thin networks are linearly stable, whereas thick networks are unstable. The critical thickness for the change in stability depends on the microscopic elastic constants. The instability is induced by the increase in the compressive load on the inner network layers as the thickness of the network increases. The here employed homogenization approach combined with more elaborate microscopic models can serve as a basis to study the evolution of polymerizing actin networks and the mechanism of actin driven motion.

15 min. break

CPP 28.5 Wed 11:45 ZEU 260

Dynamics and mechanics of formin mediated actin bundles — •Florian Rückerl, Timo Betz, and Cécile Sykes — UMR168, Institut Curie, Paris

In our experiments actin filaments and actin bundles are produced by polymerization by the formin mDia1(FH1FH2). To probe their dynamics and mechanics, we use a state of the art optical tweezers setup and create multiple traps (2 to 5) with acousto-optical deflectors (AODs). Digitally controlled AODs in time sharing mode allow to position and move several traps simultaneously. Employing a four quadrant diode as a position detector results in high temporal and spatial resolution, $10\mu s$ and <1nm, respectively. This allows to investigate the polymerizing dynamics of mDia1 by directly observing the deflection of formin coated beads inside the optical trap. Preliminary results indicate single monomer addition events at infrequent intervals.

By attaching several beads to individual bundles we can create pico-Newton forces in arbitrary directions. The mechanical properties of the bundle are then probed by bending, pushing and pulling on the bundle. We find that pulling on a bundle leads to its elongation, presumably by relative sliding of the bundle filaments to each other.

Furthermore, the setup can be used for the direct manipulation of the bundles without beads attached to it, allowing for an *in situ* non invasive measurement. Correlating the local fluctuations at several positions on the bundle yields its persistence length and gives an estimate of the number of filaments in the bundle.

CPP 28.6 Wed 12:00 ZEU 260

Network Formation of Cytoskeletal Proteins — •Christian Dammann, Bernd Nöding, Susanne Bauch, and Sarah Köster — Courant Research Centre Nano-Spectroscopy and X-Ray Imaging, University of Göttingen, Germany

The structure and function of biological systems is determined by their bio-environment. Therefore, a drop-based microfluidic device is tailored to probe context-sensitivity of biological systems. In this device a series of monodisperse aqueous drops is created and used as picoliter bio-compartments. The composition of the drops is varied from drop to drop. Thus, the biological system is encapsulated in drops with tunable chemical content. These drops are then stored in the device for long-time observations. The content composition of each individual drop can be reconstructed. Possible applications of this tool are manifold. The device proves to be suitable for *in vitro* studies on cytoskeletal proteins. We focus on the assembly and network formation of vimentin intermediate filament. The assembly of vimentin depends on the ionic strength. We are able to directly image the networks of the fluorescently tagged protein and show that divalent ions induce compaction of these networks.

CPP 28.7 Wed 12:15 ZEU 260

Functionalized lipid bilayers for rapid cell attachment — •Samira Hertrich, Martin Huth, and Bert Nickel — Ludwig-Maximilians-Universität, Department für Physik and CeNS, Geschwister-Scholl-Platz 1, 80539 München

The behaviour of cells in contact to interfaces varies significantly depending on the surface properties. Bioadhesive coatings can act as an interlayer between cells and anorganic interfaces tuning the interaction of cells with the surface. Here, a multilayer system consisting of a supported lipid bilayer and two protein layers is used to produce a surface favoring neural stem cell attachment. Biotin and streptavidin act as a layer of linkers in between the lipid bilayer and the cell adhesive polypeptide AK-cyclo[RGDfC].

The trilayer system was characterised by x-ray reflectometry (D4, HASYLAB) and neutron reflectometry (N-REX, FRM2) measurements, which allowed for the determination of the layers thicknesses and the hydration of both lipids and proteins. Cell attachment to the coated surface was verified via fluorescence microscopy [1]. Microscopy confirms rapid attachment of stem cells while reflectometry indicated a dense on edge configuration of the AK-cyclo[RGDfC] thus maximizing the number of exposed RGD groups. Experiments have been performed in collaboration with E. Madarasz and G. Menzo from the Hungarian Academy of Science (HAS).

[1] Huth, M, et al., Materials 2010, 3, 4994-5006.

CPP 28.8 Wed 12:30 ZEU 260

Two-component Polymer Scaffolds for Controlled Three-dimensional Cell Culture — •Benjamin Richter[1,2], Franziska Klein[1], Thomas Striebel[1], Clemens Franz[1], Georg von Freymann[3], Martin Wegener[2], and Martin Bastmeyer[1] — [1]Zoologisches Institut, Karlsruher Institut für Technologie, 76131 Karlsruhe — [2]Angewandte Physik, Karlsruher Institut für Technologie, 76131 Karlsruhe — [3]AG Optische Technologien und Photonik, Technische Universität Kaiserslautern, 67663 Kaiserslautern

Fibrous collagen or matrigel matrices are commonly used to study three-dimensional (3D) cell behaviour, but these matrices have a random pore size and are structurally and chemically ill defined. We and others have recently shown that direct laser writing (DLW) is a versatile technique to fabricate tailored 3D cell-culture scaffolds in the micrometer to nanometer range. By using an adequate photoresist, elastic 3D scaffolds for cell-force measurements have also been realized. These DLW scaffolds have been homogeneously coated with ECM molecules. Ideally, they should rather have an adjustable distribution of cell-substrate contact sites to manipulate cell adhesion and cell shape in all three dimensions. By sequential DLW of two different photoresists, composite-polymer scaffolds with distinct protein-binding properties are fabricated and selectively bio-functionalised thereafter. Cells cultured in these scaffolds selectively form cell-adhesion sites with the functionalised parts, allowing for controlling cell adhesion and cell shape in 3D - forming the basis for future designer tissue-culture scaffolds.

CPP 28.9 Wed 12:45 ZEU 260

Characterizing bacterial adhesion: The role of van der Waals forces — •Nicolas Thewes, Peter Loskill, Sebastian Hümbert, and Karin Jacobs — Deparment of Experimental Physics, Saarland University, 66041 Saarbrücken, Germany

Bacterial adhesion to surfaces is a complicated process that not only depends on the type of bacterium and the type of surface, but also on subsurface composition, as we have shown in a recent study. To probe the adhesion of *s. carnosus*, various surfaces have been prepared, ranging from hydrophilic to hydrophobic, from smooth to rough surfaces. To probe the effect of subsurface composition on the adhesion strength, Si wafers with different Si oxide layer thicknesses have been used. Clearly, the adhesion is stronger on wafers with thin Si oxide layer, irrespective if the wafer was hydrophobized by a monolayer of silanes or not, which is a clear evidence that long-range van der Waals forces play a crucial role for bacterial adhesion. It moreover shows that subsurface composition must be taken as characteristics of a sample, much in the same way chemical composition, wetting properties or surface roughness are taken into account. An additional parameter to control is the proper immobilization of the bacteria on the AFM tip, with the help of which force/distance curves have been performed.

CPP 29: Biopolymers and Biomaterials III (jointly with BP)

Time: Wednesday 15:00–17:45 Location: ZEU 260

CPP 29.1 Wed 15:00 ZEU 260

Spontaneous Flows of Active Polar Gels between two Rotating Cylinders — Marc Neef[1], Sebastian Fürthauer[2], •Stephan Grill[2], Frank Jülicher[3], and Karsten Kruse[1] — [1]Theoretische Physik, Universität des Saarlandes, 66041 Saarbrücken — [2]Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden — [3]Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden

Active Biological matter, e.g. cell tissues or the cytoskeleton can flow spontaneously. In situations, where the material is confined, the flow pattern depends on the geometry of the domain and the boundary conditions, as well as on the system's active properties. We investigate the influence of these factors by theoretically analyzing the equations of motion for active polar fluids in the space between two coaxial cylinders that rotate at a given frequency. In striking contrast to the behavior of uniform flows in open geometries, we find that in the confined case, activity can also stabilize uniform flow patterns.

CPP 29.2 Wed 15:15 ZEU 260

Brownian motion of stiff filaments in confined media — •Nikta Fakhri[1,4], Fred MacKintosh[2], Brahim Lounis[3], Laurent Cognet[3], and Matteo Pasquali[4] — [1]Fakultät für Physik, III. Physikalisches Institut - Biophysik , Georg-August-Universität, Göttingen, Germany — [2]Department of Physics and Astronomy, Vrije Universiteit, Amsterdam, The Netherlands — [3]Centre de Physique Moléculaire Optique et Hertzienne, Université Bordeaux, and CNRS, Talence, France — [4]Department of Chemical and Biomolecular Engineering, The Smalley Institute for Nanoscale Science and Technology, Rice University, Houston, Texas, USA

The thermal motion of stiff filaments in a crowded environment underlies the behavior of such disparate systems as polymer materials, nanocomposites, and the cell cytoskeleton. Despite decades of theoretical study, the fundamental dynamics of such systems remains a mystery. Using near-infrared video microscopy, we study the thermal diffusion of individual single-walled carbon nanotubes (SWNTs) confined in porous agarose networks. Surprisingly, we find that even a small bending flexibility strongly enhances their motion: the rotational diffusion constant is proportional to the filament bending compliance and is independent of the network porosity. This study establishes definitively the reptation dynamics of stiff filaments and provides a framework to tailor the mobility of SWNTs in confined environments.

CPP 29.3 Wed 15:30 ZEU 260

Depletion forces between single actin filaments — Martin Streichfuss[1,2], •Tamas Haraszti[1,2], and Joachim P. Spatz[1,2] — [1]Max-Planck Institute for Metals Reseach, Stuttgart, Germany — [2]Biophysical Chemistry, University of Heidelberg, Heidelberg, Germany

Filamentous actin is one of the most investigated components of the cytoskeleton in cells. The polymerization process forming the filaments from their globular actin subunits is well known to play a crucial role in cell protrusion, such as the formation of filopodia and lamellopodia.

Recent theoretical predictions suggested that the process of bundle formation of the newly polymerized actin filaments may also contribute to the forces pushing the cell membrane ahead in such protrusions. Rheology experiments reported during the last two decades on in-vitro actin gels have provided indirect information on the interactions with or without various crosslinker agents present.

We have measured the forces acting between two actin filaments using holographic optical tweezers during the bundling process in the presence of divalent cations (Mg^{2+}, 25-200 mM) or polyethylene glycol (PEG) polymer as depletion agents. The results indicate forces up to about 0.1 - 0.2 pN in a saturation manner, independent of the concentration of the magnesium ions above 50 mM.

The magnitude of these forces is comparable to the forces produced by the polymerization ratchet, providing a direct hint that the bundling forces may contribute to the formation of cellular protrusions significantly.

CPP 29.4 Wed 15:45 ZEU 260

Coarse Grained Simulations of Biopolymers: Effects of Finite Damping and Hydrodynamic Interactions — Uwe Winter and •Tihamer Geyer — Center for Bioinformatics, Saarland University, Saarbrücken

In the coarse grained Brownian Dynamics simulation method the many solvent molecules are replaced by random thermal kicks and an effective friction acting on the particles of interest. For Brownian Dynamics the friction has to be so strong that the particles' velocities are damped much faster than the duration of an integration timestep. Here we show that this conceptual limit can be dropped with an analytic integration of the equations of damped motion. In the resulting Langevin integration scheme our recently proposed approximate form of the hydrodynamic interactions between the particles [1] can be incorparated conveniently, leading to a fast multi-particle propagation scheme, which captures more of the short-time and short-range solvent effects than standard BD. Comparing the dynamics of a bead-spring model of a short peptide, we recommend to run simulations of biological molecules and polymers with the Langevin type finite damping and to include the hydrodynamic interactions [2].

[1] Geyer, Winter, *J. Chem. Phys.* **130** (2009) 114905
[2] Winter, Geyer, *J. Chem. Phys.* **131** (2009) 104102

CPP 29.5 Wed 16:00 ZEU 260

Transport of a semiflexible filament in a network — •Teresa Bauer[1], Felix Höfling[2], Erwin Frey[1], and Thomas Franosch[3] — [1]Arnold Sommerfeld Center (ASC) for Theoretical Physics and Center for NanoScience (CeNS), Fakultät für Physik, Ludwig-Maximilians-Universität München, Germany — [2]Max-Planck-Institut für Metallforschung, Stuttgart and Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany — [3]Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Germany

The cytoskeleton of a cell is comprised of a network of various biopolymers. A prominent example is the filamentous actin, a semiflexible polymer studied extensively also in vitro. The transport of a single semiflexible filament in a strongly entangled network is highly directed along the confining tube formed by the surrounding network.

We have investigated the dynamics of a semiflexible filament in a plane in the presence of immobilized obstacles mimicking the constraints of the crosslinked network. The inextensibility constraints are encoded via a bead-rod-algorithm extended by a suitable collision rule and extensive simulations are performed. In particular we quantify the translational and rotational diffusion investigated for a broad density range and visualize the dynamics using representative animations. Furthermore we discuss issues of numerical stability.

15 min. break

CPP 29.6 Wed 16:30 ZEU 260

Interplay of conformational degrees of freedom and crosslink binding in filamentous biopolymer bundles — •Claus Heussinger — Institute for Theoretical Physics, University of Goettingen, Germany

Crosslinked F-Actin bundles constitute principal components of a multitude of cytoskeletal processes and play key roles in many cellular functions. Much of the special properties of crosslinked biopolymer bundles derives from the interplay of bundle conformational degrees of freedom with the internal binding status of the crosslinking agent. Depending on probing time- and length-scales this interplay can lead to interesting dynamical effects as well as non-trivial elasto-plastic phase-behavior. By employing theoretical considerations combined with Monte-Carlo simulations, we will discuss some aspects of the internal dynamics of the cross-linker whose binding affinity serves to stabilize the bundle. We show how an imposed bundle deformation modifies the equilibrium binding constant and even allows for the coexistence of different bundle states.

CPP 29.7 Wed 16:45 ZEU 260

Interfacial effects on amyloid fibrilization — •Chiu Fan Lee[1], Létitia Jean[2], Chongsoo Lee[2], Michael Shaw[2], and David J. Vaux[2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Sir William Dunn School of Pathology, Oxford, UK

Amyloid accumulation is associated with pathological conditions, including type II diabetes and Alzheimer's disease. Lipids influence amyloidogenesis and are themselves targets for amyloid-mediated cell membrane disruption. Amyloid precursors are surface active, accumulating at hydrophobic-hydrophilic interfaces (e.g., air-water), where their biophysical and kinetic behaviors differ from those in the bulk solution with significant and underappreciated consequences. Using a combined experimental and theoretical approach, we demonstrate amyloid fibrilization is critically dependent on the presence of air-water interface (AWI). Furthermore, we showed that the role of membranes in amyloidogenesis has been previously underestimated; in an *in vivo*-like situation (with no AWI), anionic liposomes (containing dioleoylphosphatidylglycerol) enhanced islet amyloid polypeptide (IAPP) fibrillogenesis far more than described previously in conventional assay conditions (in the presence of an AWI). These findings have implications for the protein misfolding field and in assay design to target toxic protein aggregation.

Reference: L. Jean, C. F. Lee, C. Lee, M. Shaw, D. J. Vaux. FASEB J. **24**, 309 (2010).

CPP 29.8 Wed 17:00 ZEU 260

Keratin homogeneity in the tail feathers of peacocks — •Silvia Pabisch[1,2], Stephan Puchegger[1], Ingrid M. Weiss[3], Helmut O. Kirchner[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]INM-Leibniz

Institute for New Materials, Saarbrücken, Germany

X-ray diffraction studies successfully clarified the structure of avian feathers: Each filament has a helical structure with four repeating units per turn.[1] The structure of avian feathers is very stable though their relative density is low. The keratin structure in the cortex of peacocks' feathers is studied by X-ray diffraction along the feather, from the calamus to the tip. It changes considerably over the first 5 cm close to the calamus and remains constant for about 1 m along the length of the feather. We attribute the X-ray patterns to a shrinkage of a cylindrical arrangement of beta-sheets, which is not fully formed initially. In the final structure, the crystalline beta-cores are fixed by the rest of the keratin molecule. The hydrophobic residues of the beta core are locked into a zip-like arrangement. Tensile and compression tests are additionally performed in-situ to follow the structural change as consequence of varying load.

[1] R.D.B. Fraser and D.A.D. Perry, J. Struct. Biol. 162 (2008) 1-13.

CPP 29.9 Wed 17:15 ZEU 260

Thermophoresis quantifies the Conformation and Stability of Biomolecules — •Christoph Jens Wienken, Philipp Baaske, Stefan Duhr, and Dieter Braun — Systems Biophysics, LMU München, Germany

Stability and conformation of biomolecules is important in the field of biology, medical diagnostics and biotechnology. We developed a method which measures both parameters using Microscale Thermophoresis, an all-optical technique which only uses 250nl of sample. Thermophoresis is the directed movement of molecules in a temperature gradient. It depends on surface characteristics of the molecule, such as size, charge and hydrophobicity [1]. Its sensitivity for small changes in above parameters was recently shown by analyzing the binding reactions of DNA aptamers and a variety of proteins [2,3].

When measuring thermophoresis over temperature, information about the thermal stability of biomolecules are accessible. We find clear melting transitions and resolve intermediate conformational states. With this it is possible to analyze single nucleotide polymorphisms, DNA modifications and conformational states. The thermophoretic melting analysis is also applicable to proteins where unfolding patterns comparable to scanning calorimetry are found.

[1] Duhr,S & Braun,D Proc. Natl Acad. Sci. USA 103, 19678 (2006).

[2] Baaske,P et al. Angew. Chem. Int. Ed. 49, 2238 (2010).

[3] Wienken,CJ et al. Nat. Commun. 1:100 (2010).

CPP 29.10 Wed 17:30 ZEU 260

Liquid-liquid phase separation in protein solutions induced by multivalent counter ions — •Marcell Wolf, Fajun Zhang, Felix Roosen-Runge, Andrea Sauter, and Frank Schreiber — Institut für Angewandte Physik, Auf der Morgenstelle 10, Universität Tübingen, 72076 Tübingen, Germany

The liquid-liquid phase separation (LLPS) in concentrated protein solutions plays an important role for protein crystallization as well as protein-association related diseases, such as the sickle cell anemia and eye cataracts, etc [1]. Here, we show that the LLPS can be induced in protein solutions by using a multivalent salt like Yttrium Chloride (YCl_3). The phase diagram of proteins with YCl_3 in the c_p (protein concentration) - c_s (salt concentration) plane is determined. The protein solution undergoes a phase-separation upon adding salt up to a critical value c*. Further increasing c_s to c** the precipitates dissolve and the system turns back to a homogenous solution. This is a reentrant phase behavior [2]. In the condensed regime between c* and c** the system is thermodynamically equivalent to the phase behavior of a hard sphere with short range interactions, which exhibits a stable gas-solid transition and a metastable LLPS. The phase boundary is determined by UV and X-ray absorption. The effective protein-protein interactions in solutions upon LLPS are investigated by SLS and SAXS. The resulting interaction potential has been compared and discussed based on the thermodynamic criteria. [1] J.D. Gunton, A. Shiryayev, D. L. Pagan, Protein Condensation, 2007, Cambridge University Press, [2] F. Zhang et al., Phys. Rev. Lett. 101 (2008) 148101

CPP 30: Glasses and Glass Transition I (jointly with DY, DF)

Time: Wednesday 10:15–13:00 Location: KÖN Farb

CPP 30.1 Wed 10:15 KÖN Farb

Boson-peak in glasses and random-matrix statistics — •Walter Schirmacher — Institut für Physik, Univ. Mainz — Physik-Department E13, TU München

The enhancement of the vibrational density of states (DOS) with respect to the Debye expectation ("boson peak"), which is universally observed in glasses, is considered by means of of symmetry arguments. Low-frequency wave-like excitations in a disordered solids probe a homogeneous and isotropic material. Due to these symmetries the vibrational wave-like states are highly degenerate (Debye regime). This degeneracy is lifted at higher frequencies. In this regime the discretized equation of motions are governed by a sparse random matrix. The eigenvalues of this matrix are non-degenerate and show the distance statistics of the Gaussian orthogonal ensemble ("level repulsion"). It is conjectured that the integrated density of levels in this regime increases linearly. The cross-over from the Debye regime to the random-matrix regime leads in three dimensions to an enhancement of the DOS. In two dimensions this is not the case. Model calculations using a field-theoretical approach [1] and inspection of simulation data [2] confirm this reasoning.

[1] W. Schirmacher, Europhys. Lett. Europhysics Letters, 73, 892 (2006); [2] see e.g. S. K. Sarkar, G. S. Matharoo, A. Pandey, Phys. Rev. Lett. 92,215503 (2004)

CPP 30.2 Wed 10:30 KÖN Farb

Identification of facilitation effects in supercooled liquids — •Andreas Heuer and Christian Rehwald — Institute of Physical Chemistry, University of Muenster

In a first step we analyze the information content of the finite-size effects of a glass-forming system. Interestingly, the diffusion constant shows a very weak and the structural relaxation time a very strong finite-size effect [1]. This result reflects the dynamic coupling of different regions in real space via a facilitation mechanism. We can formulate a minimum model of the glass transition which can reproduce in detail the observed features of these finite-size effets. It can be regarded as a generalization of the kinetically constrained models [2].

In a second step we search for a direct evidence of this facilitation mechanism in computer simulations. Using the setup of a highly non-equilibrium configuration these causal relations between successive relaxation events can indeed be found and characterized.

[1] C. Rehwald, O. Rubner, A. Heuer, Phys. Rev. Lett. 105, 117801 (2010).

[2] Y. J. Jung, J. P. Garrahan, and D. Chandler, Phys. Rev. E 69, 061205 (2004).

CPP 30.3 Wed 10:45 KÖN Farb

Dynamics of shear transformation zones during mechanical cycling of glassy CuTi - a molecular dynamics study — •Lennart Fricke und S. G. Mayr — Leibniz-Institut fuer Oberflaechenmodifizierung, Translationszentrum fuer regenerative Medizin und Fakultaet fuer Physik und Geowissenschaften der Universitaet Leipzig, 04318 Leipzig

Plastic deformation of bulk metallic glasses at low temperatures occurs in highly localized regions, called shear-transformation-zones (STZ) [1] - as corroborated recently in detailed experimental and simulational studies. After activation, these STZs should possess a memory of their configuration prior to transformation due to confinement by the surrounding elastic matrix, i.e. the Eshelby back-stress. While this picture surely is intuitive, it is particularly interesting whether it applies in a strict or only statistical sense and up to what strain levels. With this background we study shear behavior during mechanical cycling of Cu-Ti with a maximum of 1% to 10% shear strains in large–scale MD simulations using realistic embedded atom method (EAM) potentials. Evaluating suitable quantities, including non-affine displacements and atomic-level Basinski–Duesbery–Taylor (BDT) stresses, we address the reversibility of STZs and the underlying physics on the atomic scale.

[1] A. S. Argon, Acta Metall. 27, 47 1979

This project is funded by the German DFG - PAK 63

CPP 30.4 Wed 11:00 KÖN Farb

Describing experimentally obtained stress overshoots

in sheared colloidal dispersions with schematic MCT — •Christian Peter Amann[1], Matthias Fuchs[1], Miriam Siebenbürger[2], and Matthias Ballauff[2] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Helmholtz Zentrum für Materialien und Energie, 14109 Berlin, Germany

Sheared viscoelastic media show a stress overshoot between elastic and plastic deformation regime, i.e. a maximum in the shear stress vs. strain plot after switching on a constant shear rate. We found a way to model such overshoots with the $F_{12}^{(\dot\gamma)}$ model, a schematic model of a microscopic mode-coupling theory (MCT) approach to describe glass forming liquids. The enhancement of the schematic model is tested by fitting experimental strain-stress curves from sheared colloidal dispersions of thermosensitive core-shell particles. Flow curves and linear stress response moduli of the same experimental setup could be fitted well with the $F_{12}^{(\dot\gamma)}$ model [1]. Furthermore this model has been able to describe nonlinear stress response to oscillatory shear rates [2]. The implementation of stress overshoots in this schematic model was motivated and guided by the recently identified mechanism within microscopic MCT framework causing such overshoots to occur [3]. This mechanism is also identified to be highly connected to a super-diffusive motion regime of the colloids [3].

[1] M. Siebenbürger et al., *J. Rheol.* **53**, 707–726 (2009)
[2] J.M. Brader et al., arXiv:1010.2587v1 (2010)
[3] J. Zausch et al., *J. Phys.: Condens. Matter* **20**, 404210 (2008)

CPP 30.5 Wed 11:15 KÖN Farb

Evaluation of MD force fields for ion transport in glassy materials — •Christian Trott[1], Martin Körner[1], Michael Schuch[2], and Philipp Maass[2] — [1]Theoretical Physics II, Technische Universität Ilmenau, 98684 Ilmenau, Germany. — [2]Fachbereich Physik, Universität Osnabrück, 49076 Osnabrück, Germany

Ion conducting glasses are an interesting class of materials with a wide range of possible applications, including batteries, supercapacitors, and smart windows. Considerable efforts have been undertaken to understand their properties with the help of experimental and theoretical investigations such as molecular dynamics (MD) simulations. Most of the previous MD studies of ion conducting glasses have been limited to structural analysis and the existing investigations of ion transport were almost all performed at comparatively high temperatures just below the "computer glass transition" temperature. Recent advances in hardware and MD software, namely the development of the GPU-MD code LAMMPS$_{\text{CUDA}}$, allow for a much more comprehensive investigation of long term dynamics. We assess the power of a number of interaction models for investigating long range ion transport in glasses. Specifically we determine diffusion constants and selected activation energies in several ion conducting glass systems for which force fields have been suggested in the literature.

CPP 30.6 Wed 11:30 KÖN Farb

Lorentz-like power-law decay of velocity anti-correlations in a supercooled liquid — •Felix Höfling[1] and Peter Colberg[2,3] — [1]Max-Planck-Institut für Metallforschung, Stuttgart, and Institut für Theoretische und Angewandte Physik, Universität Stuttgart — [2]Chemical Physics Theory Group, Department of Chemistry, University of Toronto, Canada — [3]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln

Harnessing the compute power of recent graphics processors, we have measured the velocity-autocorrelation function (VACF) in the supercooled Kob-Andersen mixture for large systems of 50,000 particles, providing data with an excellent signal-to-noise ratio. The emergence of glassy dynamics upon supercooling is systematically accompanied by a power-law decay of the VACF at intermediate times with exponent 5/2 and negative prefactor, similarly as observed recently for the hard sphere liquid (Williams *et al.*, PRL 2006). Such anti-correlations are reminiscent of the well-known, universal long-time tail in the Lorentz model with the same exponent and sign. The role of dynamic heterogeneities for the power-law decay is addressed by considering correlation functions that are restricted to the most mobile or immobile particles. We find that the Lorentz-like decay is absent in the VACF of the most mobile particles and conclude that the power law is *not* a manifestation of dynamic heterogeneities. For the most immobile particles, however, the power-law decay is well pronounced and we propose that the relevant mechanism is given by repeated encounters with the quasi-arrested, microscopic particle cages.

CPP 30.7 Wed 11:45 KÖN Farb

Universal jamming phase diagram in the hard-sphere limit and comparison of the dynamics of soft and hard spheres — •Michael Schmiedeberg[1], Thomas K. Haxton[2], Sidney R. Nagel[3], and Andrea J. Liu[4] — [1]Institut für Theoretische Physik 2: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany — [2]Theory of Nanostructured Materials, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA — [3]The James Franck Institute, The University of Chicago, Chicago, IL 60637, USA — [4]Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104, USA

We present a new formulation of the jamming phase diagram for a class of glass-forming fuids consisting of spheres interacting via finite-ranged repulsions. Our phase diagram is universal at low pressure, i.e. observables such as the relaxation time are insensitive to details of the interaction potential and collapse onto the values for hard spheres.

Furthermore, we show that the dynamics of soft spheres can be described in terms of the dynamics of hard spheres. By introducing an effective hard sphere diameter that is determined from the soft-sphere pair potential via the Andersen-Weeks-Chandler approximation, the relaxation times of soft spheres can be mapped onto the curve known for hard-sphere liquids. These results indicate that the dynamics of soft spheres depend on an effective free volume in a universal way.

CPP 30.8 Wed 12:00 KÖN Farb

Investigation of the dephasing of tunneling systems in glasses using two-pulse polarisation echo experiments — •Masoomeh Bazrafshan, Paul Fassl, Martin Schwarze, Angela Halfar, Annina Luck, Andreas Fleischmann, and Christian Enss — Kirchhoff Institut für Physik, Universität Heidelberg

Low temperature properties of glasses are governed by atomic tunneling systems. Many aspects are well described within the phenomenological standard tunneling model. Tunneling systems couple to their local strain fields which gives rise to a strain-mediated coupling among them. These interactions cause time-dependent variations in the energy splittings of tunneling systems when their neighbors undergo thermal transitions. This is the basis of the spectral diffusion model, which describes the dephasing of tunneling systems at very low temperatures. Experimentally, this dephasing of tunneling systems can be studied by two-pulse polarisation echo experiments. We have performed such echo decay measurements with an improved setup allowing us to observe echoes at very long delay times where the echo has decayed five orders of magnitude from its original amplitude. We have analysed the time and temperature dependent results in the framework of spectral diffusion model, finding very good qualitative agreement for the echo decay, but clear shortcoming in terms of the temperature dependence.

CPP 30.9 Wed 12:15 KÖN Farb

Structural investigations on Eu-doped fluorobromozirconate glass ceramics. — •Marie-Christin Wiegand[1], Bernd Ahrens[2], Bastian Henke[2,3], and Stefan Schweizer[2,3] — [1]Department of Physics, University of Paderborn, Warburger Str. 100, 33100 Paderborn, Germany — [2]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale), Germany — [3]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale), Germany

Modified Eu-doped fluorozirconate glasses are regarded as promising materials for photovoltaic and medical applications. In these glasses, a substantial fraction of the fluorine ions was replaced by bromine ions resulting in the formation of $BaBr_2$ nanocrystals upon subsequent thermal treatment of the as-made glass. Interestingly, the metastable hexagonal phase of $BaBr_2$ is always formed first before further annealing leads to the formation of orthorhombic phase $BaBr_2$, i.e., a phase transition from hexagonal to orthorhombic phase $BaBr_2$ occurs upon annealing. During the annealing a part of the doped Eu^{2+} is incorporated into the $BaBr_2$ nanocrystals enabling fluorescent transitions of Eu^{2+} in hexagonal and orthorhombic $BaBr_2$, respectively, upon ultraviolet excitation. The nanocrystal size and the structural phase depend on the addition of InF_3 and YF_3 and on the Br/(F+Br)-ratio, which was investigated by differential scanning calorimetry and x-ray diffraction. In addition, photoluminescence experiments were performed to monitor the phase transition by optical means.

CPP 30.10 Wed 12:30 KÖN Farb

Optical and structural properties of fluorozirconate-based glass ceramics doped with divalent and trivalent europium. — •Christian Passlick[1], Bastian Henke[1,2], Jacqueline Anne

Johnson[3], and Stefan Schweizer[1,2] — [1]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale) — [2]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale) — [3]Department of Materials Science and Engineering, University of Tennessee Space Institute, Tullahoma, TN 37388, USA

Eu-doped fluorozirconate-based glass ceramics can be used for x-ray detection in medical diagnostics as well as for down-converting top layers in photovoltaics. A modified ZBLAN composition consisting of a mixture of Zr, Ba, La, Al, and Na fluorides was additionally doped with chlorine ions to initiate the formation of $BaCl_2$ nanocrystals upon thermal treatment of the as-poured glasses. During annealing some of the Eu^{2+} ions are incorporated into the nanocrystals enabling a strong blue fluorescence upon ultraviolet excitation or x-ray irradiation. In this work, focus is put on the amount of divalent and trivalent Eu fluoride and chloride additives since it is known that the expensive Eu^{2+} can be produced by melting the cheaper Eu^{3+} raw material. Influences of the different Eu oxidation states on the $BaCl_2$ crystallization and the optical response of the glass ceramics are presented.

CPP 30.11 Wed 12:45 KÖN Farb

Multi-phonon relaxation in Eu-doped fluorozirconate-based glasses and glass ceramics — •Charlotte Pfau[1], Christian Bohley[1], Manuela Miclea[1], Paul-Tiberiu Miclea[2,3], and Stefan Schweizer[2,1] — [1]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale) — [2]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle — [3]Institute of Physics, Martin-Luther-University of Halle-Wittenberg, Heinrich-Damerow-Str. 4, 06120 Halle

Eu-doped fluorozirconate(FZ)-based glasses are of interest for various fluorescence applications such as photon down-conversion layers for high efficiency solar cells or ionizing radiation imaging plates. Multiphonon relaxation (MPR) is one of the major quenching processes of the rare-earth (RE)-related fluorescence therein. The MPR is significantly reduced in hosts providing low phonon frequencies such as FZ-based glasses and glass ceramics; the latter contain barium halide nanocrystals with even lower phonon frequencies. However, the MPR rate depends not only on the phonon frequency, but also on the electron-phonon coupling between the rare-earth ion and the host lattice. The local vibrational environment of the RE ion is investigated by phonon sideband spectroscopy. To analyze the vibrational spectra and their influence on the fluorescence properties, a series of Eu-doped FZ-based glasses and glass ceramics has been studied by Raman, phonon sideband, and fluorescence spectroscopy. The MPR rate is determined for the levels involved in the fluorescence process.

CPP 31: Organic Semiconductors IV: Excitations and Charges (jointly with HL, DS)

Time: Wednesday 14:00–17:00 Location: ZEU 222

Topical Talk CPP 31.1 Wed 14:00 ZEU 222

Control of Charge Carrier Dynamics in Disordered Conjugated Polymers — •Dirk Hertel — Physical Chemistry, University of Cologne, Luxemburgerstr. 116, 50939 Cologne, Germany,

We developed a new method to probe charge carrier mobility on ultrafast time scale [1]. It is based on electric field induced second harmonic generation. The method is applied to prototypical amorphous conjugated polymers of the polyphenylene- and polyfluorene-type. Typically the carrier mobility in these organic polymers decreases with time in a power law fashion from about 1 cm^2Vs^{-1} at 1 ps to its stationary value of about 10^{-6} cm^2Vs^{-1} in hundreds of ns.

The dynamics of the mobility is discussed. It will be shown, that in nanoscale devices the macroscopic mobility is not adequate to describe charge transport. We study the influence of disorder, morphology and temperature on ultrafast transport. At early times the transport is dominated by tunneling [2] and disorder plays already an essential role. Comparison of transient photocurrents with Monte-Carlo simulation reveals that on-chain transport has to be invoked to rationalize our results [3]. The hopping rates for intrachain transport are much larger compared with interchain transport. The results give access to essential transport properties for the development of advanced theoretical models and may help to design improved solar cells.

[1] A. Devižis, et al. *Phys. Rev. Lett.* **103**, (2009) 027404.
[2] A. Devižis, et al. *Phys. Rev. B* **82**, (2010) 155204.
[3] A. Devizis, et al. *Chem. Phys. Lett.* **498**, (2010) 302.

CPP 31.2 Wed 14:30 ZEU 222

Light-Emitting Organic Memory — •Peter O. Körner, R. Clayton Shallcross, Vincent Aubert, Eduard Maibach, Philipp Zacharias, and Klaus Meerholz — Department of Chemistry, University of Cologne

We report on light-emitting organic memory (LE-OMEM) devices composed of multiple solution-processed layers. The active layer of our LE-OMEM devices is comprised of crosslinkable dithienylethene photochromes (XDTE) that can be optically switched between two energetically distinct and thermally stable isomers. Exploiting the difference in the HOMO and LUMO levels of these two isomers we use such a layer as an electrical switch within our OLED layer stack. We demonstrate that the ON/OFF ratio in current (OOR_j) as well as in electroluminescence (OOR_L) of such devices is exponentially dependent on the difference in the largest charge injection barrier between the ON and OFF state of the device. Optimized devices displayed impressive fatigue resistance and afforded values for OOR_j and OOR_L of greater than 10^3. We focus on a variety of crosslinkable DTE molecules of varying structure and functionality with an emphasis on OOR, device stability over multiple read/write/erase cycles (fatigue resistance) and switching rates. Current induced switching allows for electrical writing and reading of grey level information in these XDTE devices. We studied this electrical switching behavior to gain further insight into the distinct switching mechanisms within the XDTE layer. These fundamental studies are a first step towards a completely electrically driven LE-OMEM.

CPP 31.3 Wed 14:45 ZEU 222

Determination of the effective radiative quantum efficiency of light-emitting guest-host systems — •Tobias Schmidt[1], Daniel-Steffen Setz[2], Benjamin Lebsanft[1], Thomas Wehlus[1], Jörg Frischeisen[1], Benjamin Krummacher[2], Michael Flämmich[3], Norbert Danz[3], and Wolfgang Brütting[1] — [1]Experimentalphysik IV, Universität Augsburg — [2]OSRAM Opto Semiconductors, Regensburg — [3]Fraunhofer-Institut für angewandte Optik und Feinmechanik (IOF), Jena

The efficiency of organic light-emitting diodes (OLEDs) is still limited as only a small part of the applied electrical power is converted into light and finally extracted from the device to air. Especially the radiative quantum efficiency (RQE) of the used guest-host system is often declared to be unity in phosphorescent emitter/matrix combinations. Due to interference effects, the radiative lifetime of the emitter and thus the effective RQE of the light-emitting guest-host system is influenced by coupling to different modes of the cavity formed by the metallic mirror and the partially reflecting ITO/glass interface. The effective RQE can be determined by measuring the external quantum efficiency of the electrically driven OLED or the photoluminescence lifetime of the emitter inside the OLED at different emitter positions in the cavity. We have investigated the RQE of the commonly used emitter $Ir(ppy)_3$ in neat films with PMMA and CBP as matrices, yielding values of about 70 %, and compare it to OLEDs, where significantly lower values of only 40 % are obtained.

CPP 31.4 Wed 15:00 ZEU 222

Exciton quenching in light emitting organic field-effect transistors studied by localized Spectroscopy — •Wouter Koopman, Stefano Toffanin, and Michele Muccini — ISMN-CNR, Via P. Gobetti 101, 40129 Bologna, Italy

The recent development of organic light-emitting transistors (OLETs) promises a new generation of light-emitting organic devices surpassing the efficiency of organic LEDs. The transistor structure prevents non-radiative processes connected to charge-carrier injection as for the ideal OLET the full recombination takes place inside the channel.

In this work we present an investigation of the influence of field-induced quenching on the luminescence intensity in OLETs based on *N,N' ditridecyl-perylene-3,4,9,10-tetracarboxylic diimide* (PTCDI-

C13H27) as a model compound. We have used localized photoluminescence and lifetime spectroscopy to study the quenching processes at the electrodes and in the channel region in working devices. Our measurements show a reduction of luminescence intensity up to 20% by applying a forward gate voltage, with a gate field in the order of $1{\times}10^{8}Vm^{-1}$. Upon application of a reverse bias a counter-intuitive enhancement of the PL spectrum was found. Excluding polaron-injection by a dielectric barrier, we can identify field induced effects to be responsible for the observed effects.

These results clarify the role of external electric field induced exciton-quenching on the luminescence efficiency of OLETs and establish a bases for the understanding of the limiting processes in more complex devices.

CPP 31.5 Wed 15:15 ZEU 222

Triplet Excimer Emission in a Series of CBP-Derivatives — •Sebastian Hoffmann[1], Pamela Schrögel[2], Rodrigo Albuquerque[1], Michael Rothmann[2], Peter Strohriegl[2], and Anna Köhler[1] — [1]Department of Physics, University of Bayreuth, 95440 Bayreuth — [2]Macromolecular Chemistry I, Department of Chemistry, University of Bayreuth, Bayreuth 95440, Germany

Carbazole-based materials such as 4,4*-bis(N-carbazolyl)-2,2*-biphenyl (CBP) and its derivatives are frequently used as matrix materials for phosphorescent emitters in organic light emitting diodes. An essential requirement for such matrix materials is a high energy of their first triplet excited state. Here we present a detailed spectroscopic investigation supported by DFT calculations on two series of CBP derivatives, where CH3 and CF3 substituents introduce strong torsion into the molecular structure. The resulting poor coupling between the two halves of the molecules leads to an electronic structure similar to that of N-phenyl-3,6-dimethyl-carbazole, with high triplet state energy of 2.95 eV. However, we also observe a triplet excimer emission centred at about 2.5-2.6 eV in all compounds. We associate this triplet excimer with a sandwich geometry of neighboring carbazole moieties. For compounds with more polar CF3 substituents, the lifetime of the intermolecular triplet excited state extends into the millisecond range for neat films at room temperature. We attribute this to an increased charge-transfer character of the intermolecular excited state for the more polar substituents. [1] S.T. Hoffmann et al, J. Phys.Chem. B, in press.

15 min. break

CPP 31.6 Wed 15:45 ZEU 222

The effect of energetic disorder on the spectral diffusion of singlet and triplet states in phenylene-type polymers — •Anna Köhler[1], Sebastian T Hoffmann[1], Heinz Bässler[1], Jan-Moritz Koenen[2], and Ullrich Scherf[2] — [1]Experimental physics II, Universität Bayreuth — [2]Macromolecular Chemistry, Bergische Universität Wuppertal

We have employed quasicontinuous temperature dependent fluorescence and phosphorescence spectroscopy to monitor the spectral diffusion of singlet and triplet excitons in a series of pi-conjugated polymers.(1) The experimental results are complemented by Monte-Carlo simulations. We investigated (i) how spectral diffusion is controlled by the degree of energetic disorder present in the amorphous film and (ii) how this process depends on the range of the electronic coupling by comparing singlet exciton diffusion via long-range Förster transfer against triplet exciton diffusion by short-range Dexter transfer. For singlets, we find that the fluorescence spectra bear out a bathochromic shift upon cooling the sample down to a critical temperature below which the shift saturates. This bathochromic shift is a signature of spectral relaxation. In contrast we observe a hypsochromic shift of the phosphorescence spectra below a characteristic temperature for triplets in systems with at least moderate energetic disorder. We show that Random-walk theory applied to excitation transport within a Gaussian density-of-states distribution is both necessary and sufficient to rationalize the experimental results in a quantitative fashion. (1) S.T. Hoffmann et al. PRB 81, 115103 (2010)

CPP 31.7 Wed 16:00 ZEU 222

Surface Doping of Conjugated-polymer/Insulating-polymer Composite Film for Field-effect-transistor — •Guanghao Lu[1,2], Patrick Pingel[2], Ingo Salzmann[1], Norbert Koch[1], and Dieter Neher[2] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany

In organic field-effect-transistors, optimized devices are usually achieved at inert environment together with passivated dielectric surface, in order to prevent the possible doping by oxygen or polar groups at dielectric surface. However, in this work, we find that the field-effect properties of poly(3-hexylthiophene)/polystyrene (P3HT/PS) composite can be greatly improved upon surface doping. Upon exposure to air and using oxidablely active dielectric surface, we doped the top surface and bottom surface of P3HT/PS film for top-contact and bottom-contact devices, respectively. The field-effect mobility of these films with only 2-5 wt% P3HT can be enhanced by more than 3 orders, reaching 0.05-0.2 cm2V-1s-1. This phenomenon is strongly contrary to the case of pure P3HT film. We proposed that, for pure P3HT, doping inevitably induces negatively charged sites or charge-transfer complexes, which act as new traps or undesired low energy sites. However, for conjugated-polymer incorporated within insulating-polymer matrix, the interaction between hole and surrounding negative sites is weaker because of the spatial occupation of a-PS among P3HT domains, which largely optimizes the positive aspect of doping and meanwhile restrained its negative role.

CPP 31.8 Wed 16:15 ZEU 222

Investigation of single grains in nanoscale P3HT OFETs — •Dileep Dhakal, Steve Pittner, Torsten Balster, and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen

Regio-regular poly(3-hexylthiophene) (P3HT) has a chain length in the range of several nm up to more than 100 nm, depending on the molecular weight. In addition, the lateral correlation length of 50 nm thick spin-coated P3HT-layers was found to be 150 nm [1] corresponding to the range of structural order within the film. Therefore, the reduction of the channel length L in organic field effect transistors towards the sub-100 nm range will open up the possibility for channels formed by single grains or individual P3HT chains. For this investigation transistor templates on oxidized silicon substrates are prepared by 2 approaches i) by electron beam lithography (EBL) and ii) by metal deposition under defined tilt angle at a preexisting contact edge. The resulting channel length between the source and drain electrode is in the range from 1 μm to 100 nm for EBL and reaches even lower channel sizes using the second approach. At L = 1 μm a mobility of 10^{-2} cm^2/Vs is typically extracted from transfer curve measurements. Without optimization of the gold/P3HT-interface we find a decrease of mobility by more than one order of magnitude for 100 nm devices, which is attributed to an increased influence of the contact resistance. The ratio can be clearly improved by optimizing the interface. [1] B. Gburek and V. Wagner, Org. Electronics 11 (2010) 814.

CPP 31.9 Wed 16:30 ZEU 222

The impact of polar bonds on electron transport through self-assembled monolayers — •David A. Egger[1], Ferdinand Rissner[1], Egbert Zojer[1], and Georg Heimel[2] — [1]Institute of Solid State Physics, Graz University of Technology, Austria — [2]Institut für Physik, Humboldt-Universität zu Berlin, Germany

Density functional theory based surface- and transport-calculations are performed to elucidate the role of intra-molecular polar bonds built into self-assembled monolayers (SAMs) sandwiched between two metal electrodes. Conjugated (oligo)phenylene-ethynylenethiols (also known as 'Tour wires') on gold are chosen due to their frequent appearance in past experimental and theoretical studies. Here, we substitute carbon by nitrogen atoms in a systematic way to realize two different molecules with zero dipole moment and virtually identical frontier molecular orbital energies. Despite this similarity in the electronic structure of the isolated species, the charge-transport characteristics of the corresponding SAMs are vastly different. We give a sound explanation for our observations based on an intuitive electrostatic rationale and conclude that the actual orientation of polar bonds in monolayers of preferentially oriented molecules crucially impacts characteristic parameters of molecular electronic devices, such as conductance gap or threshold voltage.

CPP 31.10 Wed 16:45 ZEU 222

Photoinduced magnetoresistance in organic field-effect transistors — •Thomas Reichert and Tobat P. I. Saragi — Department of Mathematics and Science and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Strasse 40, D 34132 Kassel, Germany

We report on negative magnetoresistance (MR) in low external magnetic fields in organic field-effect transistors. This effect can only be observed if the device is irradiated. MR strongly depends on gate voltage but is independent of drain voltage. Furthermore, the MR increases as the intensity of irradiation increases and the relationship of both parameters is not linear. The dependency of MR on magnetic field is not linear either, but it follows Non-Lorentian function. The triplet exciton-charge reaction model is a possible explanation for negative MR in irradiated organic field-effect transistors.

CPP 32: Transport and Spectroscopy in Molecular Nanostructures I (related to SYMN, jointly with MO)

Time: Wednesday 14:00–17:00 Location: ZEU 160

CPP 32.1 Wed 14:00 ZEU 160

Site-specific assembly of DNA-based photonic wires using programmable polyamides — Wu Su[1], •Markus Schuster[2], Clive Bagshaw[3], Ulrich Rant[2], and Glenn A. Burley[1] — [1]Department of Chemistry, University of Leicester, Leicester, UK — [2]Walter Schottky Institut, TU München, Garching, Germany — [3]Department of Biochemistry, University of Leicester, Leicester, UK

DNA constitutes a unique programmable scaffold for nanotechnological applications where the assembly of functional materials with nanoscale precision is an essential requirement. Of particular interest is the development of nanophotonic sensors and devices where DNA's addressable architecture enables the precise arrangement of fluorophores to produce an optical output. Various approaches for the construction of DNA photonic wires have been investigated; however current methods lack the ability to achieve well-defined and reproducible assemblies with high energy transport efficiency.

Here we show the construction of a site-specific, programmable DNA photonic wire model system by the utilization of fluorophore-tethered-pyrrole-imidazole polyamides (PAs) which inserts a fluorophore at a precise location within a DNA duplex. We demonstrate for the first time the construction of site-directed fluorophore assemblies along a pre-formed DNA duplex and reveal the importance of such control by the demonstration of efficient energy transport over distances in excess of 27 nm.

CPP 32.2 Wed 14:15 ZEU 160

Single molecule fluorescence-excitation and emission spectroscopy on the same individual light harvesting 2 complexes from *Rps. acidophila 10050* — •Ralf Kunz[1], Kõu Timpmann[2], Arvi Freiberg[2], Richard J. Cogdell[3], and Jürgen Köhler[1] — [1]Experimental Physics IV, University of Bayreuth — [2]Institute of Physics, University of Tartu — [3]Institute of Molecular, Cell & Systems Biology College of Medical, Veterinary and Life Sciences, University of Glasgow

Fluorescence-excitation and emission spectra from the same individual light harvesting 2 complexes from *Rps. acidophila strain 10050* measured at low temperature will be presented. The combination of both spectroscopic techniques provides information about the absorbing and emitting electronic states within the same LH2 complex.

To our surprise we find different types of emission spectra (with/without zero-phonon line) which do not correlate with different types of fluorescence-excitation spectra. The shape of the emission spectra, however, shows a clear correlation with the spectral position.

CPP 32.3 Wed 14:30 ZEU 160

Photocurrent of a single Photosystem I — •Daniel Gerster[1], Simone M. Kaniber[2], Johannes V. Barth[1], Alexander W. Holleitner[2], Itai Carmeli[3], and Joachim Reichert[1] — [1]Physik Department E20, TU München, James-Franck Str, D-85748 Garching — [2]Walter Schottky Institut and Physik-Department, TU München, Am Coulombwall, D-85748 Garching — [3]Center for NanoScience and Nanotechnology and School of Chemistry, Tel Aviv University, Israel 69978 Tel Aviv

Photosynthesis in plants and bacteria is driven by photoactive biomolecular complexes. Such photosynthetic reaction centers have evolved approximately 3.5 billion years ago, and they serve as the ultimate source of energy in the biosphere. The photosynthetic process involves an efficient conversion of solar energy to stable chemical energy. Photo-excitation of photosystem I (PS I) causes an electron transfer through a series of redox reactions. We report on the directed photo-current which is generated by a single PS I. The PS I is situated on an Au substrate, and it is electronically contacted by an apertureless scanning near-field optical microscope tip. The tip acts as a light source and counter-electrode at the same time. The PS I is covalently bound to the electronic circuit via cysteine mutation groups located at both ends of the electron transfer path.

CPP 32.4 Wed 14:45 ZEU 160

Atomistic modeling of light-harvesting complexes: dissipation, correlation and spectra — •Carsten Olbrich[1], Thomas Jansen[2], Jörg Liebers[1], Mortaza Aghtar[1], Johan Strümpfer[3], Klaus Schulten[3], Jasper Knoester[2], and Ulrich Kleinekathöfer[1] — [1]Jacobs University Bremen, Germany — [2]University of Groningen, Netherlands — [3]University of Illinois, Urbana, USA

The light absorption in light-harvesting complexes is performed by chlorophyll molecules. Recent experimental findings in some of these complexes suggest the existence of long-lived coherences between the individual pigments at low temperatures. In this context the question arises if the bath-induced fluctuations at different chromophores are spatially correlated or not. To this end we performed classical MD simulations and semi-empirical quantum chemistry calculations on some light-harvesting systems [1]. In these investigations at ambient temperatures, only weak correleted movement of the atoms and none for the sites could be observed [2]. Ensemble-averaged wave packet dynamics will be used to study the transfer of energy, i.e., excitons, in light-harvesting systems. On top of this, the same techniques can be employed to determine two-dimensional spectra which can be directly linked to experiment.

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

[2] C. Olbrich, J. Strümpfer, K. Schulten and U. Kleinekathöfer, J. Phys. Chem. B. (in press).

CPP 32.5 Wed 15:00 ZEU 160

Excitons in Molecular Aggregates with Lévy Disorder: Anomalous Localization and Exchange Broadening of Optical Spectra — •Alexander Eisfeld[1], Sebastiaan Vlaming[2], Victor Malyshev[2], and Jasper Knoester[2] — [1]MPI-PKS Dresden — [2]University of Groningen

We predict the existence of exchange broadening of optical lineshapes in disordered molecular aggregates and a nonuniversal disorder scaling of the localization characteristics of the collective electronic excitations (excitons). These phenomena occur for heavy-tailed Lévy disorder distributions with divergent second moments - distributions that play a role in many branches of physics. Our results sharply contrast with aggregate models commonly analyzed, where the second moment is finite. They bear a relevance for other types of collective excitations as well.

Phys. Rev. Lett. **105**, 137402 (2010)

CPP 32.6 Wed 15:15 ZEU 160

Size-dependent Excitonic Properties of Perylene Bisimide Aggregates — •Steffen Wolter, Franziska Fennel, Henning Marciniak, and Stefan Lochbrunner — Universität Rostock, Institut für Physik, Universitätsplatz 3, 18055 Rostock

The excitonic properties of J-aggregates made from substituted Perylene Bisimides are investigated by stationary and femtosecond spectroscopy. The high quantum yield of 82 % [1] and the recently shown long exciton diffusion length [2] make these aggregates promising candidates for applications like organic solar cells or optoelectronic switches. Here we focus on the excitonic properties in dependence of the aggregat size. Upon heating, a smooth transition from the J-aggregat to the monomer is observed in the absorption spectra. However, the emission shows a distinct minimum of the quantum yield at intermediate temperatures, indicating the existence of a weakly emitting species. Further information on this species is obtained by femtosecond pump probe and fluorescence lifetime measurements. For J-aggregates, pronounced annihilation is observed, indicating that the excitons are highly mobile. In contrast, almost no remaining annihilation dynamic remains and the fluorescence life time rises abruptly for the weakly emitting state. We discuss the possibility, that the weakly emitting state might be a short H-type aggregate.

[1] Li X.-Q., Zhang X., Ghosh S., Würthner F., Chem. Eur. J. 14, p.8074 - p.8078 (2008)

[2] Marciniak H., Li X.-Q., Würthner F., Lochbrunner S., submitted to J. Phys. Chem.

15 min. break

CPP 32.7 Wed 15:45 ZEU 160

Demonstration of an organic photonic gate — •Martti Pärs[1], Christiane Hofmann[1], Peter Bauer[2], Mukundan Thelakkat[2], and Jürgen Köhler[1] — [1]Experimental Physics IV, University of Bayreuth, 95440 Bayreuth, Germany — [2]Applied Functional Polymers, University of Bayreuth , 95440 Bayreuth, Germany

We demonstrate the function of an organic photonic gate, that consists of a photochromic switch that is covalently linked to two chromophores. As switch we use dithienylcyclopentene (DCP) that can reversibly be converted by light between two bistable states. As chromophores we employ perylene bisimide, whose fluorescence is monitored as a function of the state of the switch. We present results with respect to the modulation depth of the fluorescence, the quantum yield of the device, and its fatigue resistance.

CPP 32.8 Wed 16:00 ZEU 160

Spectral shifts and energy transfer in dye-functionalized nanostructures on silicon substrates — •Thomas Baumgärtel, Harald Graaf, and Christian von Borczyskowski — Center for Nanostructured Materials and Analytics, Institut für Physik, TU Chemnitz, 09107 Chemnitz, Germany

We use local anodic oxidation (LAO) via atomic force microscopy (AFM) to generate silicon oxide nanostructures with a height of a few nanometers and lateral dimensions below 50 nm on alkyl-terminated silicon. These structures can be selectively functionalized by anchoring optically active materials such as dye molecules or semiconductor nanoparticles via a chemical bottom-up approach. This controlled immobilization of fluorophores on a semiconductor surface with a high positioning accuracy in the nanometer regime is a promising step towards the creation of new types of optical nanoscopic devices and model systems. Especially interesting are the optical properties (e.g. spectral emission, excited state lifetime, transition dipole orientation) of the bound emitters which can show a rather large difference compared to a solution or randomly oriented molecules on a surface. These differences will be discussed as a result of the anchoring mechanism, the close proximity of the emitters to the underlying silicon, intermolecular aggregation and alignment and thus an efficient energy transfer.

CPP 32.9 Wed 16:15 ZEU 160

Förster Resonant Energy Transfer (FRET) in Orthogonal Chromophores — •Igor Pugliesi[1], Heinz Langhals[2], and Eberhard Riedle[1] — [1]LS BioMolekulare Optik, LMU München — [2]Dept. Chemie, LMU München

FRET has become a process of ubiquitous importance in chemistry and biochemistry. While proximity measurements of light absorbing and fluorescent structures still rely on the basic theory of FRET, recent results from 2D electronic spectroscopy on light harvesting complexes show, that a more refined model is required for an accurate description of this photophysical process [1]. We investigate the very principles of FRET on a set of perylene bisimide dyads by pump-probe spectroscopy, chemical variation and calculations. These dyad undergo transfer with near unit quantum efficiency although the transition dipole moments of donor and acceptor are in a perfectly orthogonal arrangement to each other in the equilibrium geometry. According to the point dipole approximation used in Förster theory no energy transfer should occur. Experimentally we do, however, observe ultrafast transfer times ranging from 1 ps up to 45 ps. With the transition density cube approach, the change of the spacer both in length and chemical character and temperature variations we demonstrate that energy transfer is enabled through low frequency ground state vibrations, which break the orthogonal arrangement of the transition dipole moments. The dyads presented here therefore are a first example that shows with extreme clarity the decisive role vibrational motion plays in energy transfer processes [2].

[1] Yuan-Chung Cheng and Graham R. Fleming, *Annu. Rev. Phys. Chem., 241*, 60, **2009**.

[2] Heinz Langhals, Andreas J. Esterbauer, Andreas Walter, Eberhard Riedle, and Igor Pugliesi, *J. Am. Chem. Soc.*, 16777, 132, **2010**.

CPP 32.10 Wed 16:30 ZEU 160

Electronic transport through organophosphonate monolayers on silicon/silicon dioxide substrates — •Achyut Bora[1], Anshuma Pathak[1], Kung-Ching Liao[2], Anna Cattani-Scholz[3], Gerhard Abstreiter[3], Jeffrey Schwartz[2], and Marc Tornow[1] — [1]Institut für Halbleitertechnik, TU Braunschweig, Germany — [2]Department of Chemistry, Princeton University, NJ, USA — [3]Walter Schottky Institut, TU München, Germany

Understanding the electronic transport through layered systems of organic functional layers on semiconductor surfaces is of major importance for future applications in nanoelectronics, photovoltaics and sensors. We have prepared self-assembled monolayers (SAMs) of 9,10-diphenyl-2,6-diphosphono-anthracene and 11-hydroxyundecyl phosphonic acid precursors on highly p-doped silicon surfaces coated with a ~1 nm SiO_2 layer. Contact angle, AFM and ellipsometry evidenced the homogeneity of the formed SAMs, and their thickness was determined to be 0.82 ± 0.07 nm and 1.13 ± 0.09 nm, respectively. We provided large area electrical contacts on top of the SAMs by a hanging Hg drop electrode. The measured I-V characteristics revealed an enhanced conductance of the aromatic vs. the aliphatic compounds, with current densities of the order of $10A/m^2$ and $0.01A/m^2$, at 0.5 V, respectively. We analyzed the data in terms of non-resonant tunneling through the combined oxide-SAM barrier and found good qualitative agreement up to 0.2 V bias. Preliminary measurements on organized bilayers of anthracene bisphosphonates that were grown using techniques of coordination chemistry will be discussed, too.

CPP 32.11 Wed 16:45 ZEU 160

Excited states dynamics of two-dimensional donor-acceptor systems — Juliane Köhler[1], •Ingo Fischer[1], Tatjana Quast[1], Johannes Buback[1], Tobias Brixner[1], and Christoph Lambert[2] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg — [2]Institut für Organische Chemie, Universität Würzburg

Since electron transfer (ET) is one of the fundamental steps in the working principle of optoelectronic devices, the aim of our work is the systematic study of the optically induced ET in donor-acceptor compounds. Our interest lies in the excited states dynamics that is associated with the subsequent back-electron transfer which can be determined by time-resolved transient absorption spectroscopy on a fs- and ps- timescale. Here, we present our recent experimental results on donor-substituted truxenones which are interpreted in the framework of the Marcus theory. As donor we chose the triarylamine because of its low reorganization energy. The truxenone itself is known to be a good acceptor and its C_3h symmetry allows the substitution of three donor branches. Hence, the ET dimension is extented from one to two. Furthermore we investigated the fluorenone which is the central building block of the acceptor to distinguish their excited state dynamics from the CT state.

CPP 33: Focused Session: Computational Polymer Physics - New Developments (jointly with DY)

Time: Wednesday 14:00–16:45 Location: MOL 213

Invited Talk CPP 33.1 Wed 14:00 MOL 213

Multiscale Simulation of Soft Matter: Challenges — •Florian Müller-Plathe — Eduard-Zintl-Institut für Anorganische und Physikalische Chemie and Centre of Smart Interfaces, Technische Universität Darmstadt, Germany

Systematic coarse-graining approaches to the simulation of soft materials are now commonplace. Structural coarse-graining can be performed by a variety of methods such as Iterative Boltzmann Inversion and Force Matching. There remain, however, substantial challenges to the coarse-grained models, such as: (i) Dynamical properties. Current structure based coarse-graining methods predict too fast mobilities. (ii) Scale-bridging between particle models (e.g molecular dynamics) and continuum models (e.g. finite elements). (iii) The application of coarse-graining techniques to real-world problems. This lecture will highlight the challenges and survey approaches to overcome them.

Invited Talk CPP 33.2 Wed 14:30 MOL 213

A self-consistent field approach for crosslinked polymer materials — •Friederike Schmid — KOMET 331, Institut fuer Physik, JGU Mainz

The Self-Consistent Field (SCF) theory is one of the most powerful approaches to studying inhomogeneous polymer melts and solutions. It is nowadays a standard method to calculate nanoscale structures at polymer-coated surfaces or at interfaces in polymer mixtures, self-organization of amphiphilic polymers, phase transitions between block copolymer mesophases, to name just a few examples. However, the original SCF theory has a major drawback: It can only treat polymeric fluids. Many polymeric materials have a network structure, which means that they respond elastically to stress and that deformations are restored. In the talk, a generalized SCF theory for networks shall be proposed. As a first application, it is used to study the effect of crosslinking on the order-disorder transition in ordered lamellar block copolymer phases.

Invited Talk CPP 33.3 Wed 15:00 MOL 213

Mechanical separation of short double stranded DNA: Effect of pulling geometry — •Sanjay Kumar — Department of Physics, Banaras Hindu University, Varanasi 221 005, India

Using the Exact Enumeration technique and Molecular Dynamics simulation, we study the influence of force on the melting of DNA. A force is applied perpendicular to the helix direction to study the DNA unzipping. The force-temperature diagram is consistent with the experiment but differs significantly with the theoretical predictions. However, when a force is applied along the helix direction, we have a situation similar to the DNA rupture. We show that the rupture force increases linearly with the chain length and approaches to the asymptotic value. This is consistent with the experiment. We also observed that the rupture force depends logarithmically on the loading rate. It was found that below a certain loading rate, rupture force decreases with temperature, whereas above it, increases with temperature. Using phenomenological argument, we explain why the rupture force has distinctively different behavior for two temperatures above and below a certain loading rate. We substantiate our argument with the simulation.

15 min. break

Invited Talk CPP 33.4 Wed 15:45 MOL 213

Soft coarse-grained models for multi-component polymer melts — •Marcus Müller — Institut für Theoretische Physik, Georg-August-Universität, Göttingen, Germany

The universal equilibrium properties of dense multi-component polymer systems can be described by minimal coarse-grained models that only incorporate the relevant interactions – connectivity along the molecular backbone, limited compressibility of the polymer liquid, and repulsion between unlike segment species – via simple potentials. In such a model an effective segment corresponds to many monomeric repeat units of a chemically realistic representation and the interactions between effective segments are soft. This large degree of coarse-graining allows for a computationally efficient description of large three-dimensional systems characterized by a large invariant degree of polymerization.

I will discuss simulation techniques for studying the structure formation in block copolymer materials and illustrate the advantages and limitations of this coarse-grained description.

Invited Talk CPP 33.5 Wed 16:15 MOL 213

Simulations of Polymer Electrolytes for Lithium-Ion Batteries Highly Accurate Polarizable Potentials — •Grant Smith — University of Utah, Salt Lake City, UT, USA

There is increasing interest in using polymer electrolytes for secondary lithium batteries due to improved safety and mechanical properties compared to conventional electrolytes based on organic solvents. In polymer electrolytes a lithium salt is dissolved in a polymer matrix. In principle molecular dynamics (MD) simulations can provide important insight into the mechanism of Li+ cation coordination and transport in polymer electrolytes, facilitating the development of materials with improved properties. Such simulations require the development of potential energy functions, or force fields, that are able to faithfully reproduce polymer-polymer, salt-polymer and salt-salt interactions. We have developed such potentials based upon high-level quantum chemistry studies of model compounds, and have found that the inclusion of polarization effects is critical in obtaining an accurate description of polymer electrolytes. I will discuss the nature of these potentials as well as insights into polymer electrolytes we have gained through extensive MD simulations utilizing them.

CPP 34: Poster: Elastomers and Gels

Time: Wednesday 17:00–19:00 Location: P2

CPP 34.1 Wed 17:00 P2

Tailoring the near-surface composition profiles of pressure sensitive adhesive films and the resulting mechanical properties — •Alexander Diethert[1], Katharina Ecker[1], Yana Peykova[2], Norbert Willenbacher[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany — [2]KIT, Inst. f. Mech. Verfahrenstechnik und Mechanik, Kaiserstraße 12, 76131 Karlsruhe, Germany

Pressure sensitive adhesives (PSAs) are used for many different applications, such as for example adhesive foils or binding materials. A prominent class of PSA films is based on statistical copolymers. In the presented work we focus on the PSA model system P(EHA-stat-MMA) consisting of the tacky monomer ethylhexylacrylate and the glassy monomer methylmethacrylate.

Recently, we observed the existence of enrichment layers of one type of monomer near the sample surface having an influence on the tackiness [1]. We extend this work towards tailoring the near-surface composition. One route is to use selectivity by exposing the samples to an atmosphere with the appropriate relative humidity. As a result, the surface content of the more polar PMMA increases with increasing humidity. The effect gets less pronounced with increasing distance from the film surface.

[1] Diethert et al, ACS Appl. Mater. Interfaces 2, 2060-2068 (2010)

CPP 34.2 Wed 17:00 P2

Computer simulation of Olympic Gels — •Jakob Fischer[1,2], Michael Lang[1], and Jens-Uwe Sommer[1,2] — [1]Leibniz Institut für Polymerforschung Dresden e.V., Hohe Straße 6, 01069 Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden

A polymer gel formed by ring polymers that are connected exclusively through topologic entanglements is called "Olympic Gel", since it resembles the structure of the Olympic Rings. Olympic gels are interesting materials for theorists, since they have the potential to study the effect of entanglements directly. One of the goals of our work is to study the formation of such materials, in particular we want to investigate whether the idea of Raphael et al. [1] (step-wise creation using different chain lengths) or of Pickett [2] (selectively reactive end-groups) are more promising for an experimental study. For comparison, "ideal" model gels will be created in the simulations by allowing the polymer strands to freely cross each other. The structure of the gel will be investigated using tools of knot theory [3] and the gel point and elasticity of the material will be estimated based on the connectivity of the rings and tube models of entangled polymers.

[1] E. Raphael, C. Gay. P.G. De Gennes, JStatPhys. 89, 111 (1997).

[2] G.T. Pickett, EuroPhysLett 76, 616 (2006).

[3] M. Lang, W. Michalke, S. Kreitmeier, JCompPhys 185, 549 (2003).

CPP 34.3 Wed 17:00 P2

Polymer dynamics and crosslink density of SBR nanocomposites containing fillers with different surface area — •Anas Mujtaba, M. Keller, S. Ilisch, H.-J Radusch, T. Thurn-Albrecht, K. Saalwächter, and M. Beiner — Faculty of Natural Sciences II & Center of Engineering Sciences, Martin-Luther-University, 06099 Halle/Saale, 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 matrix. Shear data shows that substituting high- with low-surface filler 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 matrix, however, are not much affected. Dynamic strain sweeps reveal the contribution of the filler network which breaks at large deformations. 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 results imply that the effective crosslink density of the SBR matrix is slightly decreasing if filler content or filler surface area increases. In general, our findings indicate a strong influence of filler surface area on the composite properties. The implications for the optimization of SBR based composites for tyre applications are discussed.

CPP 34.4 Wed 17:00 P2

Switching Behavior of Thermoresponsive Poly(2-oxazoline) Copolymers — •Sebastian Jaksch[1], Joseph Adelsberger[1], Anita Schulze[4], Stephan Salzinger[2], Stephan Huber[2], Rainer Jordan[2,4], Zhenyu Di[3], 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

Amphiphilic copolymers in aqueous solution exhibit a wide range of morphologies ranging from micellar and other colloidal structures to hydrogels at high concentrations. Poly(2-oxazoline)s represent a very attractive class of materials as their properties can be tuned from hydrophilic via thermoresponsive to hydrophobic by changing the side group from methyl (MOx) over *iso*-propyl (*i*PrOx) and *n*-propyl (*n*PrOx) to nonyl (NOx) with the backbone being rather polar. We present here measurements on different chain architectures.

Temperature-dependent SANS measurements were carried out at KWS 2/FRM II around the lower critical solution temperature (LCST) for P*i*PrOx homopolymer and gradient copolymers with NOx monomers in dilute solution in D2O. P*i*PrOx is soluble with swollen chainconformations below the LCST. With increasing amount of NOx monomers, the chainconformation becomes more compact. The chain size grows when the LCST is approached from below and follows a power law, indicating a critical phase transition. In all cases large aggregates are present as well.

CPP 34.5 Wed 17:00 P2

Cononsolvency in thermoresponsive PNIPAM-based block copolymers — •Gabriele De Paoli[1], Sebastian Jaksch[1], Anna Miasnikova[2], André Laschewsky[2], Peter Müller-Buschbaum[1], and Christine M. Papadakis[1] — [1]Physikdepartment, Physik Weicher Materie, TU München, Garching — [2]Institut für Chemie, Universität Potsdam, Potsdam

Thermoresponsive polymers are smart materials which have attracted great attention because of their potential applicability e.g. in controlled ultrafiltration [1]. Among these, poly(N-isopropyl acryl amide) (PNIPAM) exhibits in water a lower critical solution temperature (LCST) of ca. 32 °C. Interestingly, the insolubility can also be triggered by the addition of alcohols, which, in the pure state, are good solvents for PNIPAM [2]. This is the so-called cononsolvency phenomenon.

Herein, we report on the cononsolvency behavior of micelles formed by amphiphilic block copolymers having a long hydrophilic PNIPAM block and a short hydrophobic polystyrene block. Turbidity and dynamic light scattering experiments clearly show that methanol acts as a cononsolvent for these polymeric systems in water. Compared to the homopolymer, the amphiphilic block copolymers are unexpectedly more sensitive to the presence of methanol. Moreover, a control over the size of aggregates formed in solution is obtained by adjusting the amount of cononsolvent in the binary solutions.

[1] Y.S. Park et al., *Langmuir* **14**, 910 (1998). [2] H.G. Schild et al. *Macromolecules* **24**, 948 (1991).

CPP 34.6 Wed 17:00 P2

Mechanical properties of the thermo-responsive hydrogel PNIPAM investigated by Brillouin spectroscopy — •Johannes Wiedersich, Andreas Meier-Koll, Peter Müller-Buschbaum, and Winfried Petry — TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany

Poly(N-isopropyl acrylamide) (PNIPAM) is a thermo-responsive polymer that shows a volume phase transition at the lower critical solution temperature (LCST) around 33 °C. Below the LCST the polymer incorporates water molecules into its network. At higher temperatures the polymer network collapses and precipitates.

We investigate high frequency sound propagation and attenuation of this hydrogel system by means of Brillouin spectroscopy, covering the range from well below to well above the phase transition. We probe the structure and dynamics of the system on length scales close to the size of a solvated PNIPAM molecule and on timescales on the order of those of fluctuations of hydrogen bonds.

Both the sound velocity and acoustic attenuation increase with increasing concentration. This is attributed to a larger elastic modulus at higher concentrations and to a stronger damping of sound waves for more concentrated solutions, respectively. Deviations from purely exponential damping of sound waves are observed.

Above the LCST two phases coexist: One is water-like with respect to sound propagation, the other one displays a higher sound velocity than the homogeneous solution.

CPP 34.7 Wed 17:00 P2

A comparison of the thermoresponsive switching behavior in thin films of cyclic and linear PNIPAM — •David Magerl[1], Xing-Ping Qiu[2], Françoise Winnik[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funkt. Mat., 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 drug-delivery and sensors. Poly(N-isopropylacrylamide) (PNIPAM) is one of the most studied polymer in this context. There are very few studies of cyclic PNIPAM, although this topology is of great interest because of the absence of endgroups, which has a significant impact on the lower critical solution temperature (LCST), as reported in comparatives studies of cyclic and linear PNIPAM [1].

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 was varied and the films were characterized with x-ray reflectivity and optical microscopy. The swelling behavior of films exposed to water vapor was investigated as a function of film thickness in order to assess the influence of chain topography on the thin film behavior.

[1] Yuichi Satokawa et al., Macromolecules, 42(4), 1400-1403, (2009).

CPP 34.8 Wed 17:00 P2

Quellungsverhalten von oberflächengebundenen Mikrostrukturen — •Xiaoqiang Hou[1], Tobias König[1,2], Oswald Prucker[1] und Jürgen Rühe[1] — [1]IMTEK Institut für Mikrosystemtechnik, Universität Freiburg — [2]Institut für Experimentalphysik, Universität Potsdam

Oberflächengebundene Polymermikrostrukturen sind interessante Architekturen für Anwendungen in der Sensorik oder Aktorik, insbesondere im biomedizinischen Bereich. Besonders Interessant sind solche Systeme, die durch externe Stimuli geschaltet werden, indem die Strukturen durch Lösungsmittel quellen oder schrumpfen. Bei Mikrostrukturen ist dabei zu beachten, dass das Quellungsverhalten (QV) von oberflächengebundenen 2D-Strukturen sich fundamental von dem von freien 3D-Strukturen unterscheidet. In unserer Studie untersuchen wir das QV von oberflächengebundenen Hydrogel-Mikrostrukturen. Die Hydrogele weisen Strukturbreiten zwischen 1 und 250um und Strukturhöhen zwischen 10nm und 1um auf und sind über photolithographische bzw. Zwei-Photonen-Lithographie-Prozesse hergestellt worden. Dabei wurden Copolymere mit Dimethylacrylamid (DMAAm) als

Basiskomponente und benzophenongruppenhaltige Monomere als Vernetzerkomponente eingesetzt. Unter UV-Licht vernetzen die Polymere und werden an die Oberfläche des jeweiligen Substrats angebunden. Das QV wird mit Hilfe der Rasterkraftmikroskopie untersucht (Wassr/Luft). Dabei wird der Einfluss des Aspektverhältnises auf das Quellungsvermögen der Polymere untersucht.

CPP 34.9 Wed 17:00 P2

Energy Transfer as a Probe for Studying the Phase Transition of Oligo(ethyleneglycol) based Thermoresponsive Hydrogels — •Sahika Inal[1], Jonas David Kölsch[2], Dietmar Janietz[3], André Laschewsky[2], and Dieter Neher[1] — [1]Uni. of Potsdam, Inst. of Physics and Astronomy, 14476, Golm, Germany — [2]Uni. of Potsdam, Applied Polymer Chemistry, 14476, Golm, Germany — [3]Fraunhofer Inst. for Applied Polymer Research, 14406, Golm, Germany

Since their discovery, the thermally induced phase transition of thermoresponsive polymers have been widely studied by various techniques. At the temperature known as lower critical solution temperature (LCST), the polymer chains demonstrate a transition from a hydrated state to a collapsed structure, offering an excellent model to investigate molecular interactions at play. In the present study, we use energy transfer (RET) between a conjugated polymer nanoparticle (NP) and a dye labeled thermoresponsive polymer to monitor the coil globule transition of the polymer. The internal structure of this aqueous polymer solution is investigated by fluorescence spectroscopy and dynamic light scattering measurements. When the mixture is heated above LCST, the RET is more efficient, i.e. the ratio of acceptor to donor fluorescence intensity significantly increases. Simultaneously, the average size of the particles in the mixtures containing NPs undergoes a remarkable increase. We propose that the NPs become imbedded into the dehydrated globules of the collapsed chains of the polymer above LCST, forming larger globules and bringing the acceptor chromophores closer to the donor units attached to the polymer.

CPP 34.10 Wed 17:00 P2

Preparation and characterization of pNIPAM/Au composite particles — •Adrian Carl and Regine von Klitzing — Stranski-Laboratorium, Institut für Chemie, Technische Universität Berlin

Microgels made of pNIPAM present a well known and characterized thermoresponsive material which is swollen by water. Gold nanorods are interesting because their optical properties are a function of shape and environmental parameters. It is appealing to combine both materials, each possessing remarkable properties, to investigate the structure and response of those composites, namely gold nanoparticle decorated polymer gels. In order to do so, two different microgel batches were prepared, using a weak acid or base as comonomer. Two comonomers were used in order to study the influence of net charge of the microgel particle on the morphology of the synthesized systems. Gold nanoparticles of ellipsoidal and rod shape were synthesized within the microgels. The inorganic nanoparticles were prepared in different sizes and shapes. In the scope of our studies the influence of synthetic conditions on the morphological features of the obtained gold nanoparticles and the structure of the microgel composites was investigated. The composite microgels were characterized by DLS, TEM, SAXS and UV-VIS spectroscopy. TEM measurements were supposed to give insight into the distribution of gold nanoparticles within the microgel particle which was a central question of these investigations. A model is proposed that gives qualitative information on the composites inner morphology.

CPP 34.11 Wed 17:00 P2

Structural investigations of p-NIPAM microgels by incorporation of gold nanoparticles — •Kornelia Gawlitza[1], Matthias Karg[2], Adrian Carl[1], Paul Mulvaney[2], and Regine von Klitzing[1] — [1]Stranski-Laboratorium, Institut für Chemie, Technische Universität Berlin — [2]School of Chemistry & Bio21 Institute, University of Melbourne

Due to the reversible volume phase transition at around 32°C, poly-N-isopropylacrylamide (p-NIPAM) is interesting for applications like drug delivery and biocatalysis.[1] Due to the characteristic plasmon resonance of gold nanoparticles (NP) which is a function of the particle size and shape, another field of high research interest is owned by these metal NPs. One approach to receive information about the mesh size of p-NIPAM microgels is to incorporate metal NPs into the polymer network.[2] In our studies, we synthesized citrate stabilized spherical gold NPs with different diameters and different p-NIPAM microgels. Afterwards, we incorporated these NPs into the polymer by physical entrapment. Using transmission electron microscopy (TEM), we were able to observe different structures inside of the polymer network by changing the amount of crosslinker from 5% to 0.25%. Therefore, a model from previous studies was applied to get information of a 3D object from a 2D TEM image. The characterization of the synthesized gold NPs was done by TEM while the size of the p-NIPAM microgel particles was determined by Dynamic Light Scattering (DLS). [1] K. Kratz, T. Hellweg, W. Eimer, Polymer (2001), 42, 6531 [2] Kuang, M.; Wang, D.; Möhwald, H. Adv Funct Mater 2005, 15, 1611

CPP 34.12 Wed 17:00 P2

Isotropic and uniaxial ferrogels with Ni nanorods as magnetic phase — •Philipp Bender, Andreas Tschöpe, and Rainer Birringer — Universität des Saarlandes, Saarbrücken, Deutschland

The present study focuses on the synthesis and characterization of gelatine-based ferrogels with Ni nanorods as magnetic phase. With diameters < 64 nm and aspect ratios > 3 the nanorods are uniaxial ferromagnetic single-domain particles. In the resulting ferrogels the nanorods can rotate in field direction by applying a homogenous magnetic field, working against the mechanical torque, which is caused by the shear deformation of the gel matrix.The nanorods itself were synthesized by electro-deposition of Ni into porous alumina templates, released into aqueous dispersion by dissolution of the alumina layer and further processed to gelatine-based ferrogels. The nanorods are mechanically linked to the polymer network and exhibit - without further pretreatment - an isotropic orientation distribution. However, applying an external homogenous magnetic field during the gelation process enabled the preparation of magnetically textured ferrogels. In the current work angular-dependent static magnetization measurements were used to analyze the rotation of the nanorods in soft uniaxial ferrogels, using a hard uniaxial ferrogel as reference. The elastic properties of the corresponding isotropic ferrogel were characterized using a theoretical model, which is based on the Stoner-Wohlfarth-model.

CPP 34.13 Wed 17:00 P2

Magnetic field dependent optical transmission of ferrogels with Ni nanorods as magnetic phase — •Etienne Wagner, Philipp Bender, Andreas Tschöpe, and Rainer Birringer — Universität des Saarlandes, Saarbrücken, Deutschland

Uniaxial ferromagnetic single-domain Ni nanorods with diameters $<$ 64 nm and aspect ratios $>$ 3 were synthesized by electrodeposition of Ni into porous alumina templates. They were released by dissolution of the alumina matrix in aqueous sodium hydroxide solution (NaOH) containing additionally polyvinyl-pyrollidone (PVP) as surfactant. After a thorough washing procedure the nanorods were dispersed in bidistilled water, and mixed into gelatine solutions at 60°C. Applying a homogenous magnetic field while cooling down the solution to room temperature results in uniaxial ferrogels, where the nanorods are mechanically linked to the polymer network. When the surrounding gel matrix is soft enough, a magnetic torque enables the rotation of the nanorods in field direction. In the present study the elastic response of the Ni nanorods to an external homogenous magnetic field is analyzed via optical transmission. In particular, the rotation angle of the nanorods in field direction was determined dependent on the magnitude of the applied field for different particle densities, gelatine concentrations and gelation times.

CPP 35: Poster: Micro- and Nanofluidics

Time: Wednesday 17:00–19:00 Location: P2

CPP 35.1 Wed 17:00 P2

Lattice Boltzmann simulations of cytoplasmic streaming — •Katrin Wolff, Davide Marenduzzo, and Mike Cates — Institute for Condensed Matter and Complex Systems, University of Edinburgh, UK

We model the cytoplasm's streaming motion in giant algae cells using lattice Boltzmann simulations. The fluid motion is driven by myosin motors carrying vesicles and crawling along actin filaments which are attached to the outer part of the cytoplasm. We address how the high speeds observed in experiments can be transmitted through the cytoplasm by assuming a layer of lower viscosity at the outer wall of the simulated compartment. The bulk cytoplasm is crowded with cell organelles but modelled as a simple fluid of high viscosity appropriate for the shear experienced. The motivation behind the low-viscosity layer is the assumption that those cell contents populating the cytoplasm do not reach up to the cell wall resulting in a more dilute solution close to the wall. The low-viscosity layer is not simulated itself but incorporated into a partial slip boundary condition. We derive an expression for a single-parameter boundary condition based on the relative viscosities of the bulk cytoplasm and the thin layer close to the wall and the layer's thickness.

CPP 35.2 Wed 17:00 P2

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

Due to its inherent mesoscopic character and ease of implementation and parallelisation, the lattice Boltzmann method (LBM) has become a popular model for simulations of soft matter systems.

Earlier, a multi relaxation time lattice Boltzmann model for amphiphilic fluid mixtures was presented. This model allows to resolve some of the problems existing in the broadly used single relaxation time schemes. The code allows the simulation of binary and ternary multicomponent systems, containing (im)miscible and optionally amphiphilic fluid species.

Results of the investigation of applicability of the model to simulate fluid mixtures in porous media are presented. Interesting physical properties include diffusivity and relative permeabilities.

CPP 35.3 Wed 17:00 P2

Molecular Orientational Order Phenomena in Boundary Layers observed in Nanopore Flows — •Simon Gruener[1], Dominik Gerstner[1], Yannick D. Kervran[2], and Patrick Huber[1] — [1]Experimental Physics, Saarland University, Saarbruecken, Germany — [2]Université de Rennes 1, Rennes, France

We present measurements on the spontaneous as well as the externally induced invasion of liquids into silica monoliths (porous Vycor) permeated by a tortuous pore network with radii on the scale of a few nanometers only. The dynamics are recorded upon varying the complexity of the liquid's building blocks (mostly chain-like hydrocarbons). For the homologous series of non-polar alkanes we find boundary layers (i.e. immobile layers at the silica pore walls) composed of flat lying molecules with the thickness of one molecular diameter. However, switching to the series of polar 1-alcohols we detect a rearrangement of the molecular order in favor of pinned molecules being oriented perpendicular to the pore walls. This finding demonstrates the tendency to pair the polar hydroxyl groups of both the alcohol and the silica pore walls in order to minimize the system's overall energy. The thickness of the boundary layer suggests a slanting of the molecules possibly due to the viscous drag exerted by the liquid flow in the pore center. This work has been supported within the DFG priority program 1164, Nano- & Microfluidics (Grant No. Hu 850/2).

CPP 35.4 Wed 17:00 P2

Forced Imbibitions Experiments in 2D Porous Media. — •Michael Jung[1,2], Stefan Herminghaus[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 forced liquid imbibitions 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 different flow rates. 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 and the remaining oil saturation using high speed microscopy. The effect of various additional parameters, such as surface tension 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.

CPP 35.5 Wed 17:00 P2

Characterising residual oil saturation using X-ray micro Tomography — •Hagen Scholl[1], Kamaljit Singh[1,2], Marco Di Michiel[3], Mario Scheel[3], 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]European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble, France

We examined water imbibition in an initially oil saturated porous medium using X-ray micro tomography at the European Synchrotron Radiation Facility (ESRF, ID15). Our aim is to characterise the residual oil saturation after a complete water flood under various flow conditions. As a porous medium with well defined pore space and wettability, we use a pile of monodisperse microspheres. Glass and basalt spheres were used for water wet and oil wet systems, respectively. To easily distinguish the aqueous phase from the oily phase, we add a small percentage of ZnI2 to the aqueous phase. After a complete water flood, the final residual oil distribution was characterised for oil globules/blobs (ganglia) type, size and spatial distribution. It was observed that the final oil saturation in a water wet system was higher due to significant by-passing of several oil pore pockets, and it seems that the flow rates do not play a significant role in the residual oil saturation.

CPP 35.6 Wed 17:00 P2

Effects of concentration-dependent wettability on the statics and dynamics of droplets of mixtures and suspensions — •Desislava V Todorova and Uwe Thiele — School of Mathematics, Loughborough University, Leicestershire, LE11 3TU, United Kingdom

We discuss the behaviour of small drops of non-volatile liquid mixtures, colloidal suspensions and polymer solutions on a solid substrate. A hydrodynamic long-wave model is developed to analyze static and moving contact lines in the case of partially wetting liquids that show a concentration-dependent wettability. Thereby, Hamaker constants for mixtures are obtained employing homogenization techniques [1].

The model is used to study static drop profiles, in particular, the change of the equilibrium contact angle with mean solute concentration. Following this, we focus on sliding drops and look at the change of dynamic contact angles and drop profiles with concentration for the cases of constant and concentration-dependent viscosity. Individual drop and concentration profiles and characteristics of solution families are obtained employing numerical continuation and time simulation techniques [2].

[1] 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)

[2] E. Doedel, H.B. Keller, J.P. Kernevez, Int. J. Bifurcation Chaos 1, 493-520 (1991); P. Beltrame, U. Thiele, SIAM J. Appl. Dyn. Syst. 9, 484-518 (2010)

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

CPP 35.7 Wed 17:00 P2

Dynamic Wetting of Polyisoprene Melts with Different End Groups — •Elmar Bonaccurso[1], Chuanjun Liu[1,2], Mordechai Sokuler[1,2], Günter Auernhammer[2], and Hans-Jürgen Butt[2] — [1]Center of Smart Interfaces, TU-Darmstadt, Germany — [2]Max Planck Institute for Polymer Research, Mainz, Germany

We investigate the spreading of drops of polyisoprene melts with different end groups, methyl (PI-CH3), hydroxyl (PI-OH), and carboxyl

(PI-COOH), on hydrophilic silicon surfaces. The three polymers have the same backbone and contour length. The only difference lies in the end group. We show its influence on the dynamics of wetting. Our experimental results indicate, e.g., that spreading of PI-OH and PI-COOH is slowed down as compared to PI-CH3.

Lower contact angles are attained if the end groups strongly bind to the solid surface. Hence, the wetting capability of the polymer melt could be improved by non-covalent interfacial interactions via its end groups. The hydrodynamic model[1] applied to our measurements gives a good fit to the experimental data, but does not yield reasonable values for the apparent slip length. This suggests that additional dissipative processes are at work within the three-phase zone, which may not be omitted from the overall description. Molecular Kinetic Theory[2] (MKT) analysis indicates that strong binding of molecules to surface leads to longer relaxation times, thus to a slower spreading process [3].

[1] O.V. Voinov, J. Colloid Interface Sci. 226, 22 (2000) [2] T.D. Blake, J. M. Haynes, J. Colloid Interface Sci. 30, 421 (1969). [3] C.J. Liu et al., Langmuir, 26, 2544 (2010)

CPP 35.8 Wed 17:00 P2

Liquid Morphologies in granulates with various wettability — •Marc Schaber[1], Somnath Karmakar[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-Organisation, Bunsenstraße 10, D-37073 Göttingen — [3]European Synchrotron Radiation Facility, 6 rue Jules Horowitz, F-38000 Grenoble

Adding liquid to dry granulates causes the formation of a network of capillary bridges and complex liquid structures inside the granulates and typically a stiffening of the granulate is observed. Depending on wettability of the granulate different liquid structures are formed and lead to different mechanical properties. By means of computed X-ray tomography we explore the static three dimensional packing geometry of granulates and the emerging liquid distribution within them. As granulates we use glass and basalt microspheres and mixtures of both. The glass microspheres have a low contact and the basalt microspheres have a large contact angle for the used aqueous solution. Using time resolved X-ray tomography we furthermore explore the liquid equilibration process as function of wettability of the granulate. The found liquid redistribution and the emerging liquid structures are compared to the mechanical properties of the respective granulate with identical liquid content.

CPP 35.9 Wed 17:00 P2

Wetting of grooved elastic substrates — •Carsten Herrmann[1], Dominik Michler[2], Martin Brinkmann[2], and Ralf Seemann[1,2] — [1]Saarland University, Saarbrücken, Germany — [2]MPI DS, Göttingen, Germany

The wetting morphologies on grooved elastic substrates are considered experimentally and theoretically. The substrates are fabricated from Polydimethylsiloxane (PDMS) rubber and consist of straight parallel grooves having a rectangular shaped cross section. When liquid is deposited from the vapor phase into the grooves, the geometry of the grooves might be changed by the virtue of the capillary forces of the emerging liquid wetting morphologies. Depending on geometry and wettability of the substrate, either an attractive or repulsive force between the confining ridges of a groove results. This force leads to locally different groove geometries which are more or less attractive for the adsorbing liquid and thus a lateral ordering of the wetting morphologies occurs. We explore the lateral order and its development with time as well as the shape of the emerging liquid morphologies as function of wettability and groove geometry, i.e. the aspect ratio of both the grooves and the ridges. These experimental results are compared to results from analytical and numerical calculations minimizing the interface free energy and the bending energy of the ridges.

CPP 35.10 Wed 17:00 P2

Static Wetting Morphologies in Topographically Structured Substrates — •Stefan Bommer[1], Dominik Michler[2], Martin Brinkmann[2], and Ralf Seemann[1,2] — [1]Saarland University, Saarbrücken, Germany — [2]MPI DS, Göttingen, Germany

The different wetting morphologies of liquid confined to micron sized trapezoidal grooves are studied experimentally and theoretically. We explore the emerging equilibrium morphologies as function of groove wettability and groove aspect ratio, i.e. the ratio of groove depth to groove width. The grooves are fabricated in silicon by wet etching, whereas the slope of the side walls is given by the crystal lattice of the silicon. The wettability of the substrate is controlled by various self-assembly monolayers and fine tuned with a subsequent oxygen plasma treatment. The wetting morphologies consist of polystyrene deposited from the gas phase and imaged by scanning force microscopy in an intermitted mode. Morphology diagrams are derived analytically by minimizing the surface free energies and compared to the experimental results.

CPP 35.11 Wed 17:00 P2

Wetting behavior of Si surfaces decorated with well-defined nanopillars — •Stefan Wiedemann, Alfred Plettl, Paul Ziemann, and Kay Egloff — Institute of Solid State Physics, Ulm University

To influence the wetting behavior of Si surfaces, hexagonally ordered arrays of nanoparticles were prepared in a first step by micellar or colloidal techniques combined with photoseeding. These particles are used as etching masks during a subsequent reactive ion etching step resulting in correspondingly ordered arrays of nanopillars. This approach allows a systematic variation of the height (<180 nm), density and diameter (10 to 150 nm) of the pillars. After removing the residual etching mask, hydrophobicity of the samples was additionaly modified by coating with OTMS (Octadecyltrimethoxysilane) or a plasmadeposited fluorcarbonfilm. Such surfaces were characterized by SEM and AFM and their wetting behavior was studied by measuring advancing, static and receding contact angles of water droplets. Additionally, dewing was investigated on these nanostructures.

CPP 35.12 Wed 17:00 P2

Microparticle Separation in Droplet Based Microfluidics — •Michael Hein, Jean-Baptiste Fleury, and Ralf Seemann — Experimental Physics, Saarland University, Saarbrücken, Germany

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 se-paration 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 analysis.

CPP 35.13 Wed 17:00 P2

Droplet-based microfluidic techniques for the investigation of nucleation processses — •Birte Riechers, Frank Wittbracht, Alexander Weddemann, Thomas Koop, and Andreas Hütten — Universtät Bielefeld, Bielefeld, Deutschland

Nucleation is encountered in many different areas of research such as atmospheric cloud formation or phase transitions in production processes of materials. For many processes, however, the detailed mechanisms of nucleation and growth are not well understood. Thus it is of fundamental importance to develop experimental methods to study these mechanisms in more detail. One possibility is the utilization of microfluidic devices, because they allow the production of monodisperse droplets with varying diameters in the 50-500 micrometer size range.

The aim of this work is to establish a microfluidic device for the control of droplet size, shape and solute concentrations. The aqueous droplets produced in this manner can then be studied under external influences like temperature gradients in order to determine their nucleation rates as a function of temperature and droplet size. Hence, studying nucleation kinetics with the use of microfluidic devices may improve our understanding of the principles of nucleation processes.

CPP 35.14 Wed 17:00 P2

Experimentierkiste 'Den Geheimnissen der Flüssigkeiten auf der Spur' — •K. Jacobs, B. Jochum, F. Müller, A. Kasabova, M. Liénard, S. Grandthyll, C. Zeitz und C. Spengler — Universität des Saarlandes, Experimentalphysik, D-66041 Saarbrücken

Selbständiges Experimentieren ist ein attraktiver Weg, Schülerinnen und Schüler für Naturwissenschaften zu begeistern. Im Schulalltag fallen Einheiten zum selbständigen Experimentieren jedoch aus Gründen der Zeitknappheit oft weg. Die Experimentierkiste stellt zum Themenfeld der Physik der Flüssigkeiten einfache und robuste Versuchsaufbauten zur Verfügung. Bis zu 30 Schülerinnen und Schüler ab Klasse 8 können ohne weitere fachliche Betreuung Phänomene wie Scherverdickung, Oberflächenspannung, Viskosität erfahren, begreifen und charakterisieren. Alle Versuche sind so angelegt, dass besonders 'subjektive' Erfahrungen möglich sind, man z.B. Viskosität nicht nur als Zahl mit Einheit wahrnimmt, sondern buchstäblich begreift, wie sich eine hochviskose Flüssigkeit anfühlt. Diese Art der Experimentführung spricht auch Mädchen stark an und sorgt bei beiden Geschlechtern für eine nachhaltige Forschungserfahrung, die zu einer Wahl von naturwissenschaftlichen Neigungsgruppen animiert. Diese Experimentierkiste und eine weitere zum Thema 'Physik des Lichts' kann deutschlandweit an Schulen, Universitäten etc. versandt werden, siehe www.experimentierkiste.de. Finanzielle Unterstützung erfolgt im Rahmen des DFG-Schwerpunktprogramms SPP 1164 'Nano- und Mikrofluidik', Ja905/4.

CPP 35.15 Wed 17:00 P2

Microfluidic sorting of chiral particles — •Maria Zvyagolskaya and Clemens Bechinger — Universität Stuttgart, 2. Physikalisches Institut, Pfaffenwaldring 57, 70569 Stuttgart

Molecules of opposite chirality, so-called enantiomeres, show different binding affinity to other molecules which may lead to unwanted chemical reactions. Therefore , sorting of molecules with different chiralities is an important task in molecular biology or pharmaceutical industry. Here, we experimentally study a separation method based on hydrodynamic forces acting on chiral particles in microfluidic vortices [1]. Three-dimensional chiral particles on a length scale of micrometers are created by a photolithographic process and labelled with fluorescent dyes according to their chirality. We study the motion of such particles in microfluidic channels with different types of rotational flows and investigate how spatial distribution of particles in a vortex corresponds to its chirality.

[1] M. Kostur, M. Schindler, P. Talkner, and P. Hänggi, Phys. Rev. Lett. 96, 014502 (2006).

CPP 35.16 Wed 17:00 P2

Continuous chiral separation in a post array — •Lukas Bogunovic[1], Marc Fliedner[2], Sonja Wegener[1], Peter Reimann[2], Dario Anselmetti[1], and Jan Regtmeier[1] — [1]Experimental Biophysics & Applied Nanoscience, Faculty of Physics, Bielefeld University, Germany — [2]Condensed Matter Theory, Faculty of Physics, Bielefeld University, Germany

About one half of the drugs on the market are chiral and only 25 \% of all drugs are administered as pure enantiomers [1]. Because the human metabolism (as for all living organisms) functions in a highly chiral manner, it interacts differently with the two enantiomers. Consequently, the two forms have mostly different pharmacological activities underlining the need for preparational and analytical techniques. Traditionally, chiral selectors are used that specifically bind only one form. This approach, however, requires to identify a new selector for every new drug.

Here, we present the first enantioselective selector-free separation in a microfluidic post array using micrometer sized model particles. The post array is tilted with respect to the main channel axis breaking the symmetry. The sample is continuously introduced and the two enantiomers are deflected into different directions so that they could be collected in distinct reseroirs.

For future application, we would like to extend our device from quasi-2D to 3D and further miniaturize it to address drugs.

[1] G Gübtiz and MG Schmid Biopharamceutics & Drug Disposition 22 (2001) 291-336

CPP 35.17 Wed 17:00 P2

Single cell protein analysis via two-color UV/VIS laser induced fluorescence detection in microfluidic devices — •Lukas Galla, Dominik Greif, Dario Anselmetti, and Jan Regtmeier — Experimental Biophysics & Applied Nanoscience, Bielefeld University, Germany

In order to investigate and quantify the individual and heterogeneous cellular response, single cell analysis promises individual expression studies, which are not limited by ensemble averaging effects [1].

Upon extending our previous work on UV-LIF studies of single cells and protein separation at ultra-low analyte concentrations [2], we present a novel detection setup that allows the simultaneous recording of UV and VIS fluorescence signals at a ms timescale in microfluidic devices.

As first results we demonstrate protein fingerprints of Spodoptera frugiperda insect cells (Sf9) and chinese hamster ovary cells (CHO) in UV and VIS spectral range, demonstrating the feasibility of the parallel detection. [1] J. El-Ali et al., Nature 442, 403, (2006),[2] D. Greif et al., J. of Chromatography A 1206 (1), 83, (2008).

CPP 35.18 Wed 17:00 P2

On-chip realization of mixing and demixing nanoparticles using dielectrophoresis — •Martina Everwand, Dario Anselmetti, and Jan Regtmeier — Experimental Biophysics and Applied Nanoscience, Faculty of Physics, Bielefeld University, Germany

On-chip applications using microchannels are a very fast growing field of research. Point of care diagnostics or miniaturization of separation techniques are only two examples.

One distinct feature of microchannels is the laminar flow so that mixing of liquids and analytes is only driven by diffusion. Whereas a number of applications rely on that characteristic, procedures with different reaction partners are prohibitively slow. In order to investigate controlled reactions in a microfluidic device active mixing procedures are of key importance. In contrast to batch injection and detection strategies, which is a sequential process, and therefore very time consuming we explored continuous flow separations as one possibility to realize high throughput analysis, which allow further integration of functionalities up- or downstream of the separation.

Here, we present a continuous-flow application using electrodeless dielectrophoresis for efficient mixing and separation of 20 nm and 100 nm beads. A nano-microfluidic device was used with a constriction that reduces the channel height. The benefit of this device is that the parameters according to which the separation or mixing is performed can be adopted in real time while the device is running by tuning applied AC and DC voltages. This label-free technique is very promising for manipulation of polarizable biomolecules in continuous flow mode.

CPP 35.19 Wed 17:00 P2

Microfluidic gate using self-assembling superstructures of superparamagnetic beads — •Bernhard Eickenberg, Frank Wittbracht, Alexander Weddemann, and Andreas Hütten — Universität Bielefeld, Bielefeld, NRW, Deutschland

The use of magnetic beads for microfluidic applications has been thoroughly studied during the last decades. The permanent magnetic moment allows for the controlled manipulation by external (inhomogeneous) magnetic fields and the detection by magnetoresistive sensors. Depending on the ligands that are used for the functionalization of the bead surface, they can furthermore be bound to various biomolecules.

Recently, the formation of reconfigurable, self-assembling structures from superparamagnetic beads has attracted a lot of interest. While in the absence of a magnetic field the inter-particle coupling is eliminated by thermal excitation, the presence of a homogeneous magnetic field leads to alignment of the magnetic moments of the particles, causing attractive forces between the particles and the assembling of one-dimensional, chain-like superstructures. When the magnetic field is rotated in-plane, the chains follow the movement of the field direction and start to rotate.

Based on this method of external manipulation of bead superstructures by rotating homogeneous magnetic fields, a microfluidic gate was developed that allows to actively sort the flowing particles into one of two diverging channels. At flow velocities below 90 m/s, an efficiency of 95% was achieved. Thus, the system allows for a highly effective flow control without the need for complex microstructuring.

CPP 35.20 Wed 17:00 P2

A model for swimming active droplets — •Maximilian Schmitt[1], Shashi Thutupalli[2], Holger Stark[1], and Stephan Herminghaus[2] — [1]Institut für Theoretische Physik, TU Berlin — [2]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen

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. Experiments revealed that due to a bromination reaction, the chemical potential of the surfactant (mono-olein) increases causing the surface tension to increase locally. 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. Measurements of the flow around a swimming droplet revealed a flow field similar to that of a squirmer, which is a model for a spherical micro-swimmer with prescribed flow velocity on the surface.

In this contribution we construct a first simple model of the swimming mechanism of the active droplets. We establish a reaction-diffusion system on a sphere which comprises the bromination of the surfactants and the flux of new surfactants from the oil phase to the droplet. In a second step we want to simulate the flow field created by the surface-tension gradient and compare it to the measured flow field.

CPP 35.21 Wed 17:00 P2

Gold Capped Microparticles as Self-Propelled Switchable Swimmers — •Andreas Bregulla[1], Markus Selmke[1], Ralf Seidel[2], Michael Mertig[3], Klaus Kroy[4], and Frank Cichos[1] — [1]Molecular Nanophotonics Group, University Leipzig, Linnéstraße 5,04103 Leipzig — [2]DNA Motors Group, BioTeC, University of Tech- nology Dresden, Tatzberg 47-51, 01307 Dresden — [3]Physikalische Chemie, Mess- und Sensortechnik, Technische Universität Dres- den,Eisenstuckstr. 5 01069 Dresden — [4]Soft Condensed Matter Theory Group, University Leipzig, Vor dem Hospitaltore 1, 04103 Leipzig

Nanotechnology requires the independent transport of materials by nanoscale machinery in solution. Following this idea a number of concepts on self-propelled swimmers were realized during recent years. Most of them are based on catalytic reactions requiring fuel in the solution. Due to this such self propelled swimmers are non-switchable, they run until they are out of fuel. Further they cannot be controlled on an individual basis, thus either all swimmers run or none. Here we present a new concept based on self-thermophoretic action. A particle which is capped by a thin metal layer is heated by an laser beam causing a temperature gradient along the particle surface. This temperature gradient leads to a thermophoretic propulsion of the particle. The speed as well as the directed motion itself can be controlled on an individual particle basis and thus allows a whole set of new types of artificial micro- and nanoscale motors.

CPP 35.22 Wed 17:00 P2

Gold Nanoparticle Deposition onto a Microstructured Polymer-coated Substrate Using a Flow-Stream Technique — •Gerd Herzog[1,2], Adeline Buffet[1], Jan Perlich[1], Mottakin M. Abul Kashem[1], Matthias Schwartzkopf[1], Gunthard Benecke[1], Volker Körstgens[3], Peter Müller-Buschbaum[3], Rainer Gehrke[1], Wilfried Wurth[2], and Stephan V. Roth[1] — [1]HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany — [2]Universität Hamburg, Institut für Experimentalphysik, Luruper Chaussee 149, D-22761 Hamburg, Germany — [3]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany

Metal nanostructures are widely used in electronic components. Production of nanowires by deposition of gold nanoparticles out of a suspension via flow-stream technique onto a nanostructured polymer-coated substrate might offer an easy, cheap and fast solution for industrial application [1].

Here, we present an experiment in which a colloidal suspension of polystyrene nanoparticles in water is spin-coated onto a glass substrate which is subsequently rubbed with velvet to create micrometer-sized channels. A microfluidic device is used to let an aqueous suspension of gold nanoparticles flow across the coated substrate [2]. In situ GISAXS shows the progressive deposition of gold nanoparticles onto the substrate.

[1] E. Metwalli et al., Langmuir 2009, 25(19), 11815
[2] J.-F. Moulin et al., Rev. Sci. Instrum. 79, 015109 (2008)

CPP 35.23 Wed 17:00 P2

Influence of an electric field on the two phase flows in porous media — •Benoît Semin, Matthias Schröter, and Jean-Christophe Baret — Max-Planck Institut für Dynamik und Selbstorganisation, 37073 Göttingen, Germany

The use of an electric field to enhance oil recovery from porous media has been reported at both the sample and the field scales [1]. Here, we present an experimental study of this effect at the pore scale. To control and visualize the flow, we use microfluidic devices in which a model porous media is embedded. The latter is either an irregular array of pillars (2D) or a chamber filled with glass beads (3D). This model porous media is first filled with the wetting fluid (fluorinated oil) and then the non-wetting fluid (aqueous solution) is injected. The aqueous solution is dyed to allow for the measurement of the aqueous solution and oil saturations. An electric field is applied using electrodes patterned on the microfluidic device and the influence of the external electric field on the residual oil saturation is investigated. The coupling between the flow and the electric field can involve several physical mechanisms such as eletro-osmosis, electrowetting and dielectrophoresis [2]. The variation of the fluid properties (salt concentration, permittivity) and of the electric field (magnitude and frequency) can be used to determine the dominant mechanism on the oil retention. [1] Wittle and Bell, US Patent 7325604 (2008) [2] Tabeling, Introduction to Microfluidics (2006)

CPP 35.24 Wed 17:00 P2

Droplet-based microfluidic systems for dynamic surface tension measurements — •Quentin Brosseau and Jean-Christophe Baret — Max Planck Institute for Dynamics and Self-organization

The accurate characterization and the control of interfaces is of primary importance for various fields of research, from material sciences to cell biophysics. Although surface tension – one key parameter to describe interfaces – is a concept well defined for interfaces between pure liquids or in static conditions, many question arise with the dynamics of adsorption of surfactant molecules at the interfaces [1,2] and we are facing a lack of tools to study these dynamic processes. Our aim is to develop new tools for measurement of dynamic surface tensions [2]. The idea is to produce and flow droplets in surfactant solutions through microchannel designed to induce deformations of the droplet. These deformations are controlled by the balance of viscous stress and the surface tension [3] and will allow dynamic measurement, down to millisecond time-scale. The measurements of the increase of droplet deformation with time, shows that the surface tension is decreasing along the microchannel. After a transient phase, a steady-state is reached in which surfactant is in dynamic equilibrium with the continuous phase. The characteristic time for this process is of the order of a few millisecond. By varying both the nature of surfactant and its concentration, we will look for universal behavior governing the build up of interfaces.

[1] J. Bibette, Emulsions: basic principles Rep. Prog. Phys., 62, 969 (1999); [2] J.-C Baret & al., Langmuir, 25(11), 6088 (2009); [3] J. Cabral & al., Lab Chip, 6, 427 (2006)

CPP 36: Poster: Nanoparticles and Composite Materials

Time: Wednesday 17:00–19:00 Location: P2

CPP 36.1 Wed 17:00 P2

Gold nanoparticle deposition onto doped polyaniline thin films - an in situ investigation with a combination of μGISAXS and imaging ellipsometry — •Volker Körstgens[1], Monika Rawolle[1], Adeline Buffet[2], Mottakin Abul Kashem[2], Matthias Schwartzkopf[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany — [2]HASYLAB at DESY, 22603 Hamburg, Germany

Conducting composite materials based on polyaniline and gold have a broad range of possible applications in the fields of electronics, optics and biology. In this work the deposition of gold nanoparticles as an aqueous dispersion onto a polymer thin film is investigated. The polymer film consists of polystyrene-block-polyethylene oxide and polyaniline doped with camphorsulfonic acid. We use the unique in-situ combination of μGISAXS (grazing incidence small angle x-ray scattering with a μm-sized beam) and imaging ellipsometry [1]. It allows for a comprehensive sample characterization including the local film thickness and optical properties combined with structural information with a spatial resolution depending on the size of the x-ray beam.

This project is financially supported by BMBF grant 05KS7WO1.

[1] V. Körstgens et al., Anal. Bioanal. Chem. 396, 139-149 (2010).

CPP 36.2 Wed 17:00 P2

GISAXS Investigations of gold sputter deposition onto polystyrene colloidal crystals — •Matthias Schwartzkopf[1], Mottakin M. Abul-Kashem[1], Adeline Buffet[1], Gerd Herzog[1], Volker Körstgens[2], Jan Perlich[1], Kai Schlage[1], Peter Müller-Buschbaum[2], Ralf Röhlsberger[1], Stephan V. Roth[1], and Rainer Gehrke[1] — [1]HASYLAB at DESY, Notkestr. 85, D-22603, Hamburg, Germany — [2]TU München, Physik-Department, LS Funkt. Mat., James-Franck-Str. 1, D-85748 ,Garching, Germany

Nanocomposites are important materials for a large variety of current applications like solar cells of hybrid and colloidal multilayer [Kaune] or waveguides [Maier] in optical circuits. For their efficient production in industrial processes it is mandatory to know, how the colloidal polymer layer influences the metal film morphology and the growth kinetics during sputter deposition. Commercial available monodispersed carboxylated polystyrene spheres (cPS) were employed to deposit opal crystals as templates on silicon wafer by using temperature controlled drop casting method. The GISAXS results revealing a delayed growth of a gold skin layer by evolution of the sphere form factors and the transmission signal vanishes simultaneously. This study is showing some hints that sputtered gold atoms can diffuse into the brush-like anionic surface of the cPS spheres before growing vertical on top.

[Kaune] AMI 2009

[Maier] AM 2001

CPP 36.3 Wed 17:00 P2

Freestanding membranes with well defined nanopores — •Achim Manzke, Martin Keitsch, Fabian Enderle, Stefan Wiedemann, Alfred Plettl, and Paul Ziemann — Institute of Solid State Physics, Ulm University, D-89069 Ulm

SiO2-membranes homemade from SiO2-Si-wafers or commercial Si3N4-membranes are used as starting material. Unconventional micellar and colloidal lithography techniques are used to generate hexagonal arrays of Au and Pt nanoparticles on the membrans surface, respectively [1, 2]. Additionally, pure polystyrene particles can be etched down in size by isotropic oxygen plasma treatments [3]. Particles from all three methods are used as masks in subsequent etching steps. Combination of plasma etching, evaporation, and Ar-ion polishing techniques leads to cylindrical pores through the membrane. The micellar technique enables pore diameters from 15 to 50 nm at distances up to 130 nm. On the other hand, the colloidal method allows the fabrication of pores with diameters from 40 nm to micrometers at widely variable distances. Hence, the preparation of freestanding membranes with continuously selectable pore diameters in the nm-range will be demonstrated.

[1] G. Kästle et al., Adv. Funct. Mat. 13, 853 (2003)

[2] A. Manzke et al., Adv. Mater. 19, 1337 (2007)

[3] A. Plettl et al., Adv. Funct. Mat. 19, 3279 (2009)

CPP 36.4 Wed 17:00 P2

Determination of the intrinsic permeability of nanoparticles in composites with unknown microstructure — •Béatrice Hallouet and Rolf Pelster — FR 7.2 Experimentalphysik, Universität des Saarlandes, Campus E 26, D 66123 Saarbrücken, Germany

In general the details of the microstructure in nanocomposites are unknown. Nevertheless there is a need to determine the intrinsic properties of the dispersed phase, e.g. the permeability of nanoparticles, from the measured effective properties of the system. Due to the unknown microstructure a tentative analysis using simple mixture formulas can be highly erroneous. We present a method to extract at least a partial information about the intrinsic permeability of the particles from the measured spectra. Combining dielectric and magnetic measurements we are able to convert the magnetic spectra into lower and upper bounds for the permeability of the particles. The method applies to composites in a frequency range below the interfacial polarisation peak (MWS) and has been tested for magnetic nanocomposites (nanoparticles of magnetite dispersed in a polymer), the permeability spectra of which a ferromagnetic resonance exhibit.

CPP 36.5 Wed 17:00 P2

Structure Property Relationships of Nanocomposites based on Polyethylene and Layered Double Hydroxide — •Purv Purohit, Jesus Sanchez, and Andreas Schönhals — BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany

Nanocomposites based on Polyethylene (PE) and modified ZnAl Layered Double Hydroxides (ZnAl-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. Space resolved SAXS investigation show that the samples are homogeneous on a length scale of several cm and have a predominantly intercalated morphology. DSC and WAXS show that the degree of crystallinity decreases with the increasing content of LDH. The extrapolation of this dependence to zero estimates a limiting concentration of c.a. 40% LDH where the crystallization of PE is completely suppressed. 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 dodecylbenzene sulfonate (SDBS), which are adsorbed at the LDH layers. Therefore, analysis of the beta-relaxation provides information about the interfacial region between the LDH layers and the PE matrix. The glass transition temperature in this interfacial region is somewhat lower than for pure PE. This is accompanied by a change of the fragility deduced from the relaxation map.

CPP 36.6 Wed 17:00 P2

Dielectric and Thermal Investigation of adsorbed Poly(vinyl acetate) on Silica Particles — •Marieke Füllbrandt, Purv Purohit, and Andreas Schönhals — BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany

Dielectric Relaxation Spectroscopy (DRS) is applied in a broad frequency (10-1 - 106 Hz) and temperature range (178-423K) on samples with different amounts of polymer adsorbed on silica particles. DRS probe the interface at the polymer and silica. Two relaxation processes can be identified, one corresponding to the bulk polymer and other related to the interfacial molecules of polymer and silica where the dynamic glass transition is shifted to higher temperature due to reduced mobility.

Further investigations were done to obtain information about concentrations and bound carbonyl fractions of surface adsorbed Poly(vinyl acetate) using thermogravimetric analysis (TGA) and Fourier Transform Infrared Spectroscopy (FTIR) measurements.

CPP 36.7 Wed 17:00 P2

Segment density and coil dimensions of polymer chains anchored to solid surfaces — •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,Experimental Condensed Matter Physics — [2]TU Darmstadt,Ernst-Berl-Institute for Technical and Macromolecular Chemistry

Polymer chains tethered onto curved substrates show different conformation compared to the bulk case. We study two model systems of spherical silica (SI) and polystyrene (PS) nanoparticles, onto which PS chains are attached by grafting from process. These grafted nanoparticles are dispersed either in good solvent (THF) or in matrix (PS). By means of small angle x-ray scatering, the structure of bare and surface modified particles in solution is determined. We also use dynamic light scattering to estimate the hydrodynamic radii of bare, surface modified and PS grafted SI/PS particles in solution. Finally by contrast matching of core and solvent, small angle neutron scattering allows to investigate the conformation of PS chains grafted on the surface of SI and PS in solution or both PS grafted SI and PS in a PS matrix. This is achieved by varying grafting density and molecular weight of PS in solution, and by varying the molecular weight of PS matrix at constant grafted PS molecular weight in the matrix case.

In the latter situation, a decrease of the thickness of the grafted layer with increasing molecular weight of the matrix is found, contrary to PS grafted SI in PS matrix where no change is observed.

CPP 36.8 Wed 17:00 P2

Synthesis and characterization of silica-encapsulated nanorods — •Nina Haselmaier, Philipp Bender, Andreas Tschöpe, and Rainer Birringer — Universität des Saarlandes, Saarbrücken, Deutschland

Ni nanorods with diameters ranging from 15-30 nm and aspect ratios > 3 are uniaxial ferromagnetic single domain particles. The unique magnetic properties translate into rheological properties in colloidal dispersions with perspective applications in microbiology. However, due to the strong dipolar interaction, both steric and electrostatic stabilization are necessary to prevent the nanoparticles from agglomeration even in dilute suspensions. In the present study Ni nanorods were synthesized by current-pulsed electro-deposition of Ni into hexagonally ordered porous alumina-templates. Afterwards they were released from the templates by dissolution of the alumina layer in sodium hydroxide (NaOH), to which PVP (polyvinyl-pyrrolidone) was added as surfactant. A thorough washing procedure resulted in stable aqueous colloidal dispersions of the Ni nanorods. SEM (scanning electron microscopy) - and TEM (transmission electron microscopy) - characterization of the nanorods reveals that their surrounding PVP-layer is about 6 nm thick. The main purpose of the PVP-layer is to avoid the formation of strong aggregates in the dispersion during sample preparation. The focus of the present study was to replace the organic PVP-layer by a mechanically rigid inorganic silica shell in order to increase the potential for surface functionalization of the nanoparticles.

CPP 36.9 Wed 17:00 P2

Effect of external magnetic field on the alignment of metal-polymer nanocomposites — •Yuan Yao[1], Ezzeldin Metwalli[1], Heokmin Choe[1], Peter Busch[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany — [2]Jülich Centre for Neutron Science at FRM II, Forschungszentrum Jülich GmbH, Lichtenberstr. 1, 85747 Garching

Block copolymers embedded with magnetic nanoparticles have attracted strong interest as a method to fabricate hybrid nanocomposites for wide potential applications in functional devices. Furthermore, the control over the alignment of the nanoparticles within the polymer matrix is essential for producing well-aligned highly-oriented metal-polymer nanopatterns. Controlled alignment of block copolymers or metal-polymer composites was achieved via various methods. In this work, we have investigated the alignment of magnetic nanoparticles, which is maghemite, in poly(styrene-b-methylmethacrylate) diblock copolymer films. Films are prepared by solution casting. An external magnetic field is applied to the samples during the casting step. We have studied the emerged morphologies under the influence of both nanoparticle concentrations in the polymer film and the external magnetic field strength at different direction relative to the sample surface. The structures of the metal-polymer composite films have been characterized using optical microscopy, atomic force microscopy (AFM), and grazing incidence small angle neutron scattering (GISANS).

CPP 36.10 Wed 17:00 P2

Combinatorial synthesis and characterisation of binary plasmonic metal nanoparticles in micro fluid segment sequences — •Andrea Knauer[1], Steffen Schneider[1], Andrea Csáki[2], Wolfgang Fritzsche[2], and J. Michael Köhler[1,2] — [1]Techn. University of Ilmenau, Germany — [2]Inst. for Photonic Technologies, Jena, Germany

This work reports on the screening of optical properties of Au/Ag core/shell and multishell nanoparticles by automated stepwise variation of reactant ratios in two and three dimensional parameter spaces during the micro continuous-flow synthesis under segmented-flow conditions. The optical properties of binary metal nanoparticles shift with the layer ratio of the metallic components as well as with their shape, size, surface charge and ligand-shell. Therefore, the optimization of the optical properties is a multi parameter problem demanding for new experimental strategies. The complete space of the combinations of the reactant concentrations was covered by combined slowly shifting flow rates for two reactants and a periodically fast shifting flow rate of a third solution. The total flow rate was kept constant. For these synthesis screenings, the concentrations of metal salts, reducing agent, and added ligands were varied. The three-dimensional addressing of parameter spaces can be used for finding the optimal conditions for a narrow size distribution of the obtained nanoparticles and for a tuning of their optical properties.

CPP 36.11 Wed 17:00 P2

Silver nanowires grown within tubular J-aggregates — Dörthe M. Eisele[1], Holm Kirmse[1], •Egon Steeg[1], Keith J. Stevenson[2], David A. Vanden Bout[2], Stefan Kirstein[1], and Jürgen P. Rabe[1] — [1]Humboldt-Universität zu Berlin, Germany — [2]University of Texas at Austin, USA

It was shown previously that silver nanowires with diameters below 10 nm and length exceeding microns can be grown within tubular J-aggregates by reduction of silver salt [1]. The J-aggregates self assemble from amphiphilic cyanine dyes in aqueous solutions. The silver ions are reduced by oxidizing the dyes.

We report here on the formation of sliver nanowires within the aggregates under various experimental conditions. Since the nucleation is supposed to be photo-assisted the growth is influenced by the choice of illumination time and wavelength of light. Additionally, the growth kinetics plays an important role. We discuss the correlation between these parameters and the structural properties of the wires, such as diameter, length, and crystallinity. These experiments give insight into the nucleation and growth mechanism of metal nanowires within an amphiphilic template in an aqueous environment.

[1] D.M. Eisele, H. v. Berlepsch, C. Böttcher, K.J. Stevenson, D.A. Vanden Bout, S. Kirstein, and J.P. Rabe, JACS 132 (2010) 2104.

CPP 36.12 Wed 17:00 P2

TiO_2-Ag nanocomposites for antimicrobial and photocatalytic application — •Tomislav Hrkac[1], Venkata Sai Krian Chakravadhanula[1], Natalie Wohner[1], Bodo Henkel[1], Thomas Strunskus[1], Vladimir Zaporojtchenko[1], Rainer Podschun[2], Claudia Röhl[3], Dieter Garbe-Schönberg[4], and Franz Faupel[1] — [1]Institute for Materials Science - Multicomponent Materials, Christian-Albrechts-University Kiel (CAU) — [2]Institute for Infection Medicine, CAU Kiel and University Medical Center Schleswig-Holstein Campus Kiel (UKSH) — [3]Institute of Toxicology and Pharmacology for Natural Scientists, UKSH Kiel — [4]Institute of Geosciences, CAU Kiel

Nanocomposites offer the possibility to combine the antimicrobial property of Ag with the photocatalytic activity of TiO_2 in one material. Here TiO_2-Ag 3D nanocomposites with different filling factor and different morphologies were prepared by physical vapor deposition techniques. The antimicrobial and toxicological properties were studied and correlated to the silver release measured by ICP-MS. The optical and structural properties of the composite were characterized by UV-Vis, XRD, HRTEM and XPS, and the photocatalytic activity was determined by UV illuminated dye photodegradation. Considering the different morphologies the correlation of antimicrobial efficiency and silver release will be discussed.

CPP 36.13 Wed 17:00 P2

Photothermal Correlation Spectroscopy on Gold Nanoparticles and Nanorods — •Jonas Buchmann[1], Markus Selmke[1], Daniel Rings[2], Klaus Kroy[2], and Frank Cichos[1] — [1]Institut für Experimentelle Physik I, Universität Leipzig, Deutschland — [2]Institut für Theoretische Physik, Universität Leipzig, Deutschland

Photothermal Correlations Spectroscopy (PhoCS) is a detection technique that is based on the release of heat from absorbing nano-objects. The released heat changes the local temperature and the local refractive index to provide an efficient scattering of a probe laser. Thus, absorbing particles diffusing through a the focal volume create signal burst which allow the characterization of the Brownian motion of heated particles - so called hot Brownian motion.

Here we explore the hot Brownian motion of gold nano particles and gold nano rods of various sizes. Among other effects we find an anomalous size dependence of the diffusion coefficient at constant incident heating power, which is explained within the theoretical framework of hot Brownian motion.

CPP 36.14 Wed 17:00 P2

Fine-Tuning of the Plasmon-Resonance of Gold Nanoparticles in Layered Geometry — •Madlen Klötzer[1], Steffen Mitzscherling[1], Mareike Kiel[1], and Matias Bargheer[1,2] — [1]Institut für Physik und Astronomie, Universität Potsdam — [2]Helmholtz Zentrum Berlin, Berlin

Multilayer systems containing gold nanoparticles and polyelectrolytes with a high degree of structural perfection are prepared by spin assisted layer-by-layer deposition. X-ray reflectivity and TEM measurements show well stratified layers of polyelectrolytes and gold nanoparticles.(1) The particle's packing density in-plane is verified by AFM measurement. The in-plane particle distance is varied by the adsorption time of the gold suspension and the distance between the gold layers is defined by the number of polyelectrolyte double layers. Optical spectroscopy (reflection and transmission) with polarized light reveals a tuning of the particles plasmon resonance determined by the interaction of particles.

(1) M. Kiel, S. Mitzscherling, W. Leitenberger, S. Santer, B. Tier-

sch, T. K. Sievers, H. Möhwald, and M. Bargheer, Langmuir 2010, 26 (23), 18499

CPP 36.15 Wed 17:00 P2

Detection of a surface charge on fluorescent CdSe/ZnS Quantum Dots in Toluene — •Nicole Amecke and Frank Cichos — Molecular Nanophotonics, University of Leipzig, Leipzig, Germany

Semiconductor nanocrystals, that fluoresce in the visible range like CdSe/ZnS QDs, have been a widely studied material over the last decades due to applications in bio-labeling, laser diodes, solar cells and many others. Their size-tunable fluorescence shows high quantum yields, however most synthesized single crystals still show fluctuating and interrupted emission. Those effects have been mostly assumed to be due to charges in the crystal core or at the surface leading to non-radiative decay channels and spectral shifts. However, those charges remain difficult to investigate during fluorescence detection. We took another step to change this, using a confocal microscope and investigating the fluorescence intensity of QDs in a homogeneous electric field close to one electrode. We find motion to the negative electrode and the formation of a screening layer. Despite the positive charge on these particles we measure a fluorescence lifetime comparable to that of immobilized single particles. Thus, a charge in the core can be excluded. As we are measuring in toluene, an intrinsic surface charge is suggested. We estimate the amount of this charge and the percentage of charged particles by comparing velocities and concentrations with simple electrophoretic dynamics. The possibility for this charge as origin of the measured intensity fluctuations of immobilized particles is discussed.

CPP 36.16 Wed 17:00 P2

The accurate estimation of power law exponents in terms of binned data — •André Heber, Nicole Amecke, and Frank Cichos — Molecular Nanophotonics, University of Leipzig, Leipzig, Germany

Since the first observations of single quantum dots, is has been known that they show random intensity switches between a photon-emitting state, called on-state, and an off-state, where no photons are emitted. The durations of the states are described as cut-off power laws or pure power laws, respectively. It is estimated that the power laws stretch from the fluorescence lifetime of a quantum dot to hours. However, due to experimental limitation, in intensity time traces only on- and off- states longer than 1 ms can be measured. In this poster we argue that it is difficult to conclude from the measurement of binned data to the microscopic mechanisms of the blinking behavior. We compare different analysis methods including least square fits and maximum likelihood estimators of simulated blinking traces. As a result we show that linear least square fits to log-log histograms are better suited to determine the power law from binned data than maximum likelihood estimators.

CPP 36.17 Wed 17:00 P2

Competition between diffusion and aggregate formation on a single molecule level — •Frank Gerlach, Daniel Täuber, and Christian von Borczyskowski — Chemnitz University of Technology, Optical Spectroscopy and Molecular Physics, Chemnitz, Germany

Nanoparticles and dye molecules are widely used as fluorescence labels in biophysical and medical applications. For this reason the mutual interaction among these two types of reporter molecules is of special interest. In this communication we use fluorescence and single molecule methods to explore the competition between diffusion of single dye molecules in thin liquid films and aggregate formation between surface attached colloidal semiconductor quantum dots (QD) and perylene bisimide dye molecules. This is a combined study on aggregate formation [1] and diffusion experiments [2]. We observe the diffusion with respect to the competition of the dynamics in thin liquid films with aggregate formation. The formation of assemblies is a sequence of attachments and detachments, which is controlled by the ligands present on the QD surface.

[1] D. Kowerko, J. Schuster, N. Amecke, M. Abdel-Mottaleb, R. Dobrawa, F. Würthner, C. von Borczyskowski, PCCP, 12, 4112, 2010.

[2] D. Täuber, C. von Borczyskowski et al: Diff. Fund. 11, 107, 2009.

CPP 36.18 Wed 17:00 P2

Comparative studies of the electrical behavior of catalytically grown scrolled graphene and multi-walled carbon nanotubes — •Andreas Schaper[1], Mingsheng Wang[2], Houqing Hou[3], Yoshio Bando[2], and Dmitri Golberg2[2] — [1]Center for Materials Science, Philipps University, 35032 Marburg, Germany — [2]National Institute for Materials Science, Tsukuba, Ibaraki 3050044, Japan — [3]Chemistry College of Jiangxi University, Nanchang, JX 330027, P.R. China

Besides the well known single-walled and nested-tube multi-walled carbon nanotubes (SWCNTs, MWCNTs), and the successful isolated flat graphene, scrolled graphene (carbon nanoscrolls, CNSs) has been receiving increasing interest in recent time. Here, we report in situ electron microscope measurements of the electrical behavior of CNSs and CNTs prepared using catalyst-assisted chemical vapour deposition. In the low-bias region, strictly linear IV characteristics were observed with resistance values in the range 0.8 - 15.0 kΩ for CNSs and 20 - 30 kΩ for MWCNTs. With increasing applied voltage, a superlinear behavior was detected with maximum current-carrying capacities of 8.5 x 10^8 A/cm^2 (CNSs) and 10^7 A/cm^2 (MWCNTs). As revealed by the IV data and by time-resolved image sequences, the electric breakdown of the scrolls always occurred in an abrupt manner, while the nanotubes showed a sequential destruction of the concentric-shell geometry. Due to their superb properties, CNSs are promising as electronic device elements with no limitations as to electric contacting.

CPP 36.19 Wed 17:00 P2

Photoinduced Charge Transfer in Blends of PbSe Nanocrystals and Poly(3-hexylthiophene) — •Elena Selishcheva, Florian Witt, Niklas Trautwein, Holger Borchert, Jürgen Parisi, and Joanna Kolny-Olesiak — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory (EHF), 26111 Oldenburg, Germany

Colloidal, infrared-absorbing lead selenide nanocrystals (PbSe NC) are one of the promising candidates for application as a photoactive component in hybrid solar cells due to their ability to absorb light over a large energy range of the solar spectrum. The nanoparticles blended with a conjugated polymer, such as poly(3-hexylthiophene) (P3HT), are a donor/acceptor system, which can promote efficient charge transfer. The charge separation between donor and acceptor can be studied by electron paramagnetic resonance (EPR), which detects the unpaired spin of polarons, and by photoinduced absorption spectroscopy (PIA), which monitors the change in the transmission of a nanoparticles/polymer blend due to polaronic transitions.

In this work we present a novel synthesis of oleic acid capped PbSe NC. Prior to mixing with the polymer these particles were treated with hexylamine, because its shorter hydrocarbon chain (compared to oleic acid) is supposed to improve the charge transfer in blends PbSe NC/P3HT. The charge separation was studied by EPR and PIA. These measurements suggest that charges are produced by photoinduced charge transfer. The blends PbSe NC/P3HT were used to prepare first laboratory solar cells.

CPP 36.20 Wed 17:00 P2

Structural investigation of poly(organosiloxane) nanocapsules with iron oxide cores by (A)SAXS and XRD — •Johannes Möller[1], Martin A. Schroer[1], Michael Paulus[1], Patrick Degen[2], D.C. Florian Wieland[1], Christoph J. Sahle[1], Alexander Nyrow[1], Melek Cebi[2], Sabine Leick[2], 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

We report the results of (anomalous) small angle X-ray scattering ((A)SAXS) and diffraction (XRD) measurements to study the internal structure and the formation process of poly(organosiloxane) nanocapsules filled with iron oxide cores of different sizes. The synthesis of the nanocapsules has two essential features. First iron oxide nanoparticles are synthesized by a chemical precipitation process. The second step consists of the preparation of a thin poly(organosiloxane) shell around the iron oxide core. The possibility of removing partially or completely the magnetic core of the capsules by chemical etching processes offers the opportunity of assembling hollow nanocapsules, which can be used to produce new types of microreactors or for therapeutic delivery of drugs, genes or radionuclides. The radius distribution functions of the iron oxide cores are determinded by SAXS measurements, showing the dissolution of the cores inside the capsules. Information about the structure of the iron oxide cores and the poly(organosiloxane) network at the surface are revealed by X-ray diffraction.

CPP 36.21 Wed 17:00 P2

Gold Nanoparticles Decorated with oligo(ethylene glycol) Thiols: Surface Charges and their Influence on Protein Resistance — •Moritz Schollbach[1], Maximilian W. A. Skoda[2], Robert M. J. Jacobs[3], Fajun Zhang[1], and Frank Schreiber[1] — [1]IAP Universität Tübingen — [2]ISIS Rutherford Appleton Laboratory UK — [3]CRL University of Oxford UK

Protein resistant behavior of oligo(ethylene glycol) thiol self assembled monolayers (OEG SAM) on gold surfaces [1] makes them interesting for various applications. In previous studies we investigated the resistance to adsorption of bovine serum albumin (BSA) on a model system of OEG SAM coated gold nanoparticles (AuNP) [2]. Gold colloids allow easy observation because protein repulsion leads to aggregation via a depletion-attraction effect [3]. By extending this study to other proteins, we found that surface charges play a crucial role. Zeta potential (ζ) measurements of AuNP show negative values, corresponding to a low net negative surface charge. Added negatively charged protein (BSA) does not change ζ. The size distribution, obtained by dynamic light scattering (DLS), shows separate peaks for colloid and BSA. In contrast, adding the positive charged Lysozyme (LYZ) raises ζ, resulting in a charge inversion for higher LYZ concentrations. For samples with $\zeta \approx 0$ the size distribution shows aggregates of AuNP. These results indicate that LYZ can adsorb on the AuNP, neutralizing the surface charge and destabilizing the system. [1] F. Schreiber, J. Phys.: M. 16, 2004, R881. [2] F. Zhang et al. J. Phys. Chem. A, 111, 2007, 12229 [3] F. Zhang et al. Eur. Biophys. J., 37, 2008, 551

CPP 36.22 Wed 17:00 P2

Aggregationsprozesse mono- und multivalent stabilisierter Goldnanopartikel und Quantenpunkte — •Benjamin Stein und Christina Graf — Insitut für Chemie und Biochemie FU Berlin Takustr. 3 14195 Berlin

Die unterschiedlichen Aggregationsgeschwindigkeiten von Nanopartikeln, die mit mono- oder multivalent bindenden Liganden stabilisiert sind, wurden bei verschiedenen pH-Werten und Temperaturen untersucht. Die Liganden bestehen aus Thiol-terminierten Verbindungen und sind zudem durch eine Polyethylenglykoleinheit hydrophil und dadurch im pharmazeutischen Bereich vielfach anwendbar. Zunächst wurden die Austauschreaktionen an einfach zu synthetisierenden und stabilen, Citrat stabilisierten Goldnanopartikeln durchgeführt (d=17nm). Anschließend wurden die Experimente auf CdSe/ZnS-Kern-Schale-Quantenpunkte (d=4 nm) erweitert. Das Ausmaß der Aggregation der Goldpartikel wurde anhand der Lage und Breite des Plasmonenresonanzbanden im UV-Vis-Spektrum bestimmt. Zeitabhängige Messungen bei niedrigen und hohen pH-Werten zeigen, dass divalente Liganden den Aggregationsprozess gegenüber monovalenten Liganden verlangsamen. Zudem weisen die divalent geschützten Goldnanopartikel eine größere Stabilität bei erhöhten Temperaturen auf. Auch die Aggregation der Quantenpunkte bei unterschiedlichen pH-Medien, die mittels Fluoreszenz und UV-Spektren detektiert wurde, zeigt denselben Trend, dass divalente Liganden stabilisierender als monovalente wirken.

CPP 36.23 Wed 17:00 P2

Ion transport mechanisms 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, Universität Münster, Corrensstraße 30, 48149 Münster, Germany — [2]NRW Graduate School of Chemistry, Corrensstraße 36, 48149 Münster, Germany

Electrolytes based on mixtures of lithium salts and poly(ethylene oxide) (PEO) are important candidates for modern lithium ion batteries used in electronic devices. Unfortunately, in case of the common binary electrolytes like PEO/lithium-bis(trifluoromethane sulfonimide) (LiTFSI), the ionic conductivity is too low for technological use. Among several other attempts that have been made to overcome this deficiency, the incorporation of room temperature ionic liquids (RTILs) into these materials promise 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. Based on these experimental findings, we study the underlying microscopic transport mechanisms by means of MD simulations. The transport mechanisms are discussed in context with our insights from a previous study of the binary PEO/LiTFSI electrolyte, thus pointing out the microscopic processes relevant for macroscopic ion transport.

CPP 36.24 Wed 17:00 P2

Lithium-containing diblock copolymer thin films for solid-state micro-batteries — •William Hefter[1], Ezzeldin Metwalli[1], Man Nie[1], Volker Körstgens[1], Jan Perlich[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany — [2]HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany

The ion-conducting polymer electrolyte in thin film format is important in the fabrication of lightweight and shape-flexible solid-state micro-batteries. Thin hybrid films based on polystyrene-block-polyethylene oxide and the alkali salt of lithium (bis) trifluoromethanesulfonimide are investigated using optical microscopy, atomic force microscopy and grazing incidence small angle x-ray scattering. The structure of the hybrid films are examined as a function of Li/PEO ratio. Below a critical concentration cLi/PEO the crystallization of PEO is prohibited and nanostructured block copolymer films with Li incorporated in the PEO domain are obtained. In a concentration regime above cLi/PEO aggregation of Li salt to the polymer film surface occurs due to limited capability of the PEO to accommodate the Li ions in the thin film geometry. A solvent vapor annealing of such films further enriches Li salt at the surface due to the interaction with the interfaces.

CPP 37: Poster: Heterogeneous Nucleation and Microstructure Formation (related to SYMF)

Time: Wednesday 17:00–19:00 Location: P2

CPP 37.1 Wed 17:00 P2

Crystallization of charged macromolecules — •Kai Kratzer and Axel Arnold — Institut für Computerphysik, Universität Stuttgart

The crystallization of charged macromolecules has a number of important applications in many fields, such as biology, pharmacology or materials design. For example, proteins are crystallized for purification or structure determination and colloidal crystals are promising candidates for photonic crystals. However, the crystallization of proteins or colloids is still more an art rather than a technique due to the poor understanding of the underlying physical mechanisms. To create defect-free crystals (or to prevent their growth), it is necessary to know the microscopic details of the onset of crystal growth, namely the nucleation. This process is described by the classical nucleation theory (CNT) as a balance of surface tension between liquid and crystal and the crystal's lower chemical potential. We performed computer simulations of the nucleation process to gain a better understanding of how charges carried by the macromolecules and the presence of neutralizing salt and precipitation agents influence nucleation. Since nucleation is a rare event, it is inaccessible to brute force computer simulations. We succeeded in this challenge by using the Forward Flux Sampling (FFS) method, which has only recently become available. We present first FFS results on systems of charged macromolecules in the presence of an explicit salt. This will help in developing a closed theory of protein and colloidal crystallization and thereby making targeted crystallization possible.

CPP 37.2 Wed 17:00 P2

Heterogeneous nucleation at a flat wall in a colloidal model system of charged spheres — •Andreas Engelbrecht, Rafaella Meneses, and Hans Joachim Schöpe — Staudingerweg 7, 55099 Mainz

The physical and chemical properties of solidified crystalline materials depend in a crucial way from the conditions of crystal nucleation. In order to improve the conditions of production processes and even to develop novel materials with extraordinary properties a detailed knowledge of the nucleation process is most desired.

We studied the kinetics of wall induced heterogeneous nucleation in colloidal model systems of charged spheres as function of undercooling determining nucleation rate densities, crystal growth velocities and the resulting micro structure. Applying classical concepts we extract key parameters of the nucleation process giving us the possibility to characterize the competition homogeneous and wall induced heterogeneous nucleation.

Classical theories of heterogeneous nucleation predict a reduction of the nucleation barrier height, which only depends on the contact angle of the crystal nucleus. We investigated the nucleation barrier height and its dependency on the undercooling in the system. Those results were compared with microscopic investigations of the contact angle.

CPP 37.3 Wed 17:00 P2

Gauging the Phase Field Crystal Model on Simple Systems: Hard Spheres — Marco Berghoff[1], Britta Nestler[1], •Martin Oettel[2,3], and Tanja Schilling[4] — [1]Institute of Materials and Processes, Karlsruhe University of Applied Sciences and Institute of Reliability of Components and Systems, Karlsruhe Institute of Technology — [2]Institut für Physik, Universität Mainz — [3]Material- und Prozesssimulation, Universität Bayreuth — [4]Theory of Soft Condensed Matter, Universite du Luxembourg

The Phase Field Crystal (PFC) Model is a simple Landau-type free energy model for a density-like order parameter which exhibits a phase diagram with spatially constant liquid phases and crystal phases in which the order parameter periodically varies. Supplemented with diffusive dynamics, a wealth of time-dependent processes involving crystal-liquid interfaces are describable. However, precise matching of the PFC model parameters to an actual material is difficult. Here we discuss the gauging of the model to the soft matter system of hard spheres (HS) for which both reliable simulation and density functional results exist. It is found that the HS density functionals cannot be straightforwardly mapped to the PFC free energy. As a result, crystal-liquid interface tensions and growth properties can be compared only qualitatively.

CPP 38: Poster: Colloids and Complex Liquids

Time: Wednesday 17:00–19:00 Location: P2

CPP 38.1 Wed 17:00 P2

Hydration and Protein Interactions in Concentrated Electrolyte Solutions Studied by SANS — •Fajun Zhang[1], Maximilian W. A. Skoda[2], Robert M. J. Jacobs[3], Philip Callow[4], Henrich Frielinghaus[5], Vitaliy Pipich[5], Sylvain Prevost[6], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Germany — [2]ISIS, Rutherford Appleton Laboratory, UK — [3]CRL, University of Oxford, UK — [4]Institut Laue Langevin, Grenoble, France — [5]Jülich Centre for Neutron Science at FRM II, Garching, Germany — [6]Helmholtz Center Berlin, Germany

Proteins are commonly found in relatively concentrated salt solutions during protein crystallization and purification. The exact interplay of the hydration shell, the salt ions, and protein-protein interactions under these conditions are far from understood on a fundamental level, despite the obvious practical relevance. We have studied a model globular protein (bovine serum albumin, BSA) in concentrated salt solutions by SANS. By comparing with previous studies using SAXS [1], a hydration level of 0.37 g/g protein is determined. The forward intensity determined from Guinier analysis is used to determine the second virial coefficient, A_2, which describes the overall protein interactions in solution. It is found that A_2 follows the reverse order of the Hofmeister series. These effects are further discussed by comparing the contribution from the excluded volume. SANS data are further analyzed on the full q-range using liquid theoretical approaches, which is consistent with A_2 and the experimental structure factor. [1] F. Zhang, et al., J. Phys. Chem. B 2007, 111, 251.

CPP 38.2 Wed 17:00 P2

Static and Dynamic Crowding Effects from Charge- to Sterically Stabilized Protein Solutions — •Fabio Zanini[1,3], Marco Heinen[2], Felix Roosen-Runge[1], Fajun Zhang[1], Marcus Hennig[1,3], Tilo Seydel[3], Gerhard Nägele[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, Jülich, Germany — [3]Institut Laue Langevin, Grenoble, France

We have investigated static and dynamic properties of aqueous solutions of bovine serum albumin (BSA) in an integrated conceptual framework, combining static and dynamic light scattering (SLS/DLS) and small-angle X-ray scattering (SAXS) with colloid theory. We focus on solutions with sodium and calcium chloride, which are physiologically relevant and well-suited for effective modelling. Using a new theoretical approach, we are able to reproduce the measured collective diffusion constant and structure factor, up to volume fractions of 5-10% [1]. By tuning the ionic strength, we quantify the effect of macromolecular crowding along the crossover from charge- to sterically stabilized protein solutions. Moreover, we test the validity of various generalized Stokes-Einstein equations (GSE), which connect osmotic compressibility, diffusion constant, and viscosity of complex liquids. We find that, despite their appealing simplicity, the GSE schemes fail to capture the essential richness of macromolecular collective diffusion. [1] M. Heinen *et al.*, J. Appl. Cryst., 2010, 43, 970-980.

CPP 38.3 Wed 17:00 P2

Pressure Dependence of the Interaction Potential of Protein Solutions — •Martin Schroer[1], Jonas Markgraf[2], Florian Wieland[1], Christoph Sahle[1], Johannes Möller[1], Michael Paulus[1], Metin Tolan[1], and Roland Winter[2] — [1]Fakultät Physik / DELTA, TU Dortmund, Maria-Goeppert-Mayer-Str. 2, 44227 Dortmund (Germany) — [2]Fakultät Chemie, Physikalische Chemie I, TU Dortmund, Otto-Hahn Str. 6, 44227 Dortmund (Germany)

Pressure, one of the fundamental thermodynamic variables, allows to change in a controlled and reversible way the intermolecular interactions of proteins in solution without the major perturbations produced by changes in temperature or chemical composition. Moreover, hydrostatic pressures are also relevant for understanding life under extreme conditions, as for instance in exobiological or deep sea environments (where organisms have to cope with pressures up to ~1 kbar). Hence, studying protein-protein interaction as a function of pressure will give a deeper insight into the high stability of dense protein solutions (as they occur intracellularly) in biosystems living under hydrostatic pressure conditions. We present recent results of the influence of pressure on the structure and protein-protein interaction potential of dense protein solutions studied using small angle X-ray scattering (SAXS).

CPP 38.4 Wed 17:00 P2

Small Angle Scattering of Triglyceride Nanosuspensions — •Martin Schmiele[1] and Tobias Unruh[2] — [1]Technische Universität München, Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM-II), Lichtenbergstr. 1, D-85747 Garching — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Lehrstuhl für Kristallographie und Strukturphysik, Staudtstraße 3, D-91058 Erlangen

Colloidal suspensions of triglyceride nanocrystals are considered as potential drug delivery carriers in modern pharmaceutical technology. The main focus of our group lies on tripalmitin nanocrystals stabilized with phospholipids in an aqueous dispersion medium. While the mesoscopic structure of such dispersions is well studied [1] the structure of the stabilizer layer in the interface between the particles and the dispersion medium is not. It will be demonstrated that it is possible to gain detailed information about the structure of the stabilizer layer by simultaneous analysis of SAXS and SANS data. For this purpose the X-ray powder pattern simulation analysis [2] was extended to be used for neutron data as well. In the talk the simulation method will be introduced and a comparison of recent experimental and simulation results will be presented. [1] T. Unruh, H. Bunjes, K. Westesen, M.H.J. Koch. Colloid Polym. Sci. 279, 398 (2001) [2] T. Unruh. J. Appl. Cryst. 40, 1008 (2007)

CPP 38.5 Wed 17:00 P2

Experimental Observation of Colloidal Micelles — •Daniela Kraft[1], Ran Ni[2], Michiel Hermes[2], Kisun Yoon[3], David Weitz[3], Alfons van Blaaderen[2], Marjolein Dijkstra[2], and Willem Kegel[1] — [1]Van't Hoff Laboratory for Physical and Colloid Chemistry, Debye Institute for NanoMaterials Science, Utrecht University, The Netherlands — [2]Soft Condensed Matter Group, Debye

Institute for NanoMaterials Science, Utrecht University, The Netherlands — [3]Experimental Soft Condensed Matter Group, SEAS, Harvard University, USA

Colloidal particles have often been used as analogues of atoms for studying for example crystallization and are widely anticipated as ideal candidates in bottom-up assemblies with rationally designed properties. So far, super-structures such as crystals were determined mainly by the particle shape due to centrosymmetric interactions. Site-specific interactions, so called patchy interactions, between colloids may open up new and exciting assembly possibilities.

Here, we present an experimental realization of such site-specific patchy attractions between complex colloids through depletion interactions, and apply the technique to the most simple case of colloids with one patch. Such colloids with one attractive patch form clusters that resemble surfactant micelles. We discuss the similarities between the observed colloidal clusters and surfactant micelles and compare the results to computer simulations. A theoretical micelle model is used to quantify the results.

CPP 38.6 Wed 17:00 P2

Forces of Interaction within Single Pairs of Polymer-grafted Colloids as Measured by Optical Tweezers

— •Mahdy M. Elmahdy[1,3], Alla Synytska[2], Christof Gutsche[1], Gustavo Dominguez-Espinosa[1], Astrid Drechsler[2], Petra Uhlmann[2], Manfred Stamm[2], and Friedrich Kremer[1] — [1]Institute of Experimental Physics I, Leipzig University, Linnéstrasse 5, 04103, Leipzig, Germany — [2]Leibniz Institute of Polymer Research Dresden, Hohe Str. 6, 01069 Dresden, Germany — [3]Department of Physics, Mansoura University, Mansoura 35516, Egypt

Optical Tweezers are ideal tools to measure the interaction forces between polyelectrolyte-grafted colloids. Using this technique, the forces of interaction within single pairs of poly(acrylic acid) (PAA) and poly(2-vinylpyridine) (P2VP)-grafted colloids are measured as a function of concentration, valency as well as pH of the surrounding medium [1,2]. The PAA- and P2VP-grafted colloids data are quantitatively described by the Jusufi model for spherical polyelectrolyte brushes. The transition from an osmotic to the salted brush regime is observed in both polyelectrolytes. In the salted brush regime, power law dependence with an exponent of 0.3 is found, in good agreement with scaling laws. For the PAA-grafted colloids, the brush height increases with increasing pH while the P2VP-grafted colloids show a transformation in the conformation of the brushes.

References [1] Elmahdy et al., Macromolecules 2009, 42, 9096. [2] Dominguez et al., Polymer 2008, 49, 4802.

CPP 38.7 Wed 17:00 P2

Confocal Microscopy of Colloidal Aggregates under Shearing

— •Jennifer Wenzl, Miao Wang, Marcel Roth, and Günter K. Auernhammer — Max-Plack Institut für Polymerforschung, Ackermannweg 10, D-55128 Mainz

Colloidal dispersions show a rich variety of phenomena and can therefore also act as model systems for granular matter. To infer the macroscopic behavior of granular material from interactions between single particles, detailed informations about the mechanical and structural properties are necessary. This is realized in particular with a large translational shear between parallel plates with simultaneous observation by a confocal microscope. Therewith we obtain three dimensional coordinates and trajectories of every particle in the imaged volume with high resolution. The shearing is done via a piezo-controlled cell, which enables the positioning of the shear plates with nanometer accuracy. The sample thickness is variable up to 160 μm on a micrometer scale and can be verified by confocal images. As a model system we use fluorescent core-shell silica particles in cis-decaline, as they show a weak aggregation. In this presentation we address the following questions. How do particles or aggregates deform under shear or compression? Do particles slide past each other or do they roll off under external shearing forces? How are forces transmitted in colloidal films?

CPP 38.8 Wed 17:00 P2

Micro-rheology on colloids using Optical Tweezers

— •Christof Gutsche, Tim Stangner, Mahdy M. Elmahdy, Olaf Ueberschär, Carolin Wagner, and Friedrich Kremer — Institute of Experimental Physics I, Leipzig University, Linnéstrasse 5, 04103, Leipzig, Germany

Optical tweezers are experimental tools with extraordinary resolution in positioning (+/- 2 nm) a micron-sized colloid and in the measurement of forces (approx. 50 fN) acting on it - without any mechanical contact. This enables one to carry out a multifold of novel experiments. In the following forces within single pairs of colloids in media of varying concentration and valency of the surrounding ionic solution will be presented.

CPP 38.9 Wed 17:00 P2

Interactions between polymers and curved surfactant layers

— •Andreas Weber, Shun Yu, Tinka Spehr, and Bernd Stühn — Institut für Festkörperphysik, TU Darmstadt

We study the interaction between polymers and curved surfactant layers in microemulsions in the droplet phase, where surfactant stabilized droplets of water are dispersed in a matrix of oil. To study the difference between ionic and non-ionic surfactants we use either an ionic surfactant (AOT) or a non-ionic surfactant (C12E5, Brij®30). First, we examine the phase diagram of water-in-oil droplets without polymer. This is done by small angle X-ray scattering (SAXS) and light transmission experiments, where the turbidity point and thus the stability of the microemulsion is measured as a function of temperature. Then, to investigate the interaction between polymer and the curved surfactant layer, we add the hydrophilic polymer Polyethylene glycol (PEG). The location of the PEG inside the droplet is predicted to depend on the nature of the surfactant: While the PEG is expected to adsorb to the layer of the ionic surfactant AOT, in non-ionic microemulsions the PEG is supposed to be located in the water core away from the surfactant layer. SAXS is used to investigate the structure of the polymer loaded micelles and possible deformations of the droplets, dynamic light scattering and dielectric spectroscopy provide information concerning the dynamics of the droplets and the surfactant interface.

CPP 38.10 Wed 17:00 P2

Efficiency boosting in application: The influence of Poloxamers on skin friendly microemulsions for decontamination

— •Sebastian Höhn[1], Ralph Neubauer[1], Christoph Schulreich[1], and Thomas Hellweg[2] — [1]Physikalische Cemie 1, Universität Bayreuth, Deutschland — [2]Physikalisch und Biophysikalische Chemie (PC III), Universität Bielefeld, Deutschland

Bicontinuous microemulsions based on sugar surfactants are the promising media for decontamination. Various toxic chemicals and most chemical warfare agents are hydrophobic while most degradation agents are hydrophilic. Microemulsions offer an oil and a water phase, separated by a huge internal interface which allows interaction of the enzymes with the warefare agents. One limiting factor for applications is the high demand of surfactant to form stable microemulsions. By adding small amounts of amphiphilic diblock copolymers the surfactant efficiency is dramatically enhanced (efficiency boosting effect). In this contribution the influence of different commercially available triblock copolymers (Poloxamers) on two systems is shown. Due to the fact, that the added block copolymers are part of the amphiphilic interface, where the decontamination takes place the influence of different polymers on the interfacial film is of high interest. Therefore, we investigate the model system based on n-decyl-β-D-maltoside ($C_{10}G_2$) and cyclohexane by SAXS and SANS. In order to compare this model system with a technical system we changed to Simulsol SL55 ($C_{10-12}G_{1.3}$, Seppic). Upon addition of small amounts of poloxamer an increase of the surfactant efficiency is observed.

CPP 38.11 Wed 17:00 P2

Water in Reverse Micelles Studied by Neutron Scattering

— •Tinka Spehr[1], Bernhard Frick[2], Isabelle Grillo[2], and Bernd Stühn[1] — [1]Institut für Festkörperphysik, TU Darmstadt — [2]Institut Laue-Langevin, Grenoble, France

We performed neutron scattering studies on water-in-oil droplet microemulsions based on the anionic surfactant AOT to investigate the effect of micelle size on the dynamics of water. First we studied the structure and the self dynamics of the droplets as a function of temperature and composition. Using small-angle neutron scattering and elastic scans on neutron backscattering (BS) we characterized the microemulsion structure and its stability. We find that the droplets are stable down to temperatures where the contained water is deeply supercooled [1],[2]. Neutron-spin-echo was then used to determine the bending elasticity of the surfactant film and the diffusion coefficient of the entire droplets in the oil matrix [2]. Finally we focussed on the water dynamics inside droplets of two different sizes, $\omega = 3$ (8) corresponding to $R = 7$ (12) Å, combining neutron time-of-flight and BS. The average mobility of the confined water is slowed down compared to bulk water. Inside bigger droplets we observed two dynamically separated water fractions - probably corresponding to bound shell water and bulk-like core water - whereas in smaller droplets all water appears to be closely bound [3]. Wide-angle X-ray scattering is used to monitor ice formation inside the droplets. [1] T. Spehr *et al.*, Phys. Rev. E **79** (2009), 031404; [2] T. Spehr *et al.*, J. Phys.: Condens. Matter **20** (2008), 104204; [3] T. Spehr, PhD Thesis, TU Darmstadt (2010)

CPP 38.12 Wed 17:00 P2

Transparent superhydrophobis surfaces made out of hybrid raspberry-like particles — •Doris Vollmer, Maria d'Acunzi, Lena Mammen, Xu Deng, and Hans-Jürgen Butt — Max Planck Institute for Polymer Research

We report a novel method to prepare superhydrophobic films from raspberry-like particles. The term raspberry refers to the topography of the surface of the hybrid particles, which consists of a micrometer-sized polystyrene core and a rough silica shell. Multilayers of particles are formed by evaporation of the aqueous dispersant. Mechanical stability can, for example, be induced by exposure of the multilayer to a good solvent for the polymer core. Polystyrene leaks out of the core and forms bridges between the particles. The films are hydrophobized by silanization with a semifluorinate silane. Films show static contact angle for water of about 160° and roll-off angle of a few degree. Furthermore, we discuss the mechanical stability of the coatings and show how to render them transparent.

D'Acunzi, L. Mammen, M. Singh, X. Deng, M. Roth, G.K. Auernhammer, H.-J. Butt, and D. Vollmer, Faraday Discussion, 146, 35-48, 2010

CPP 38.13 Wed 17:00 P2

Hydrodynamics of colloidal suspension under external force in a narrow channel in 2D — •Fatemeh Tabatabaei — Institute for Solid State, Research Center Juelich, 52428 Juelich, Germany

Investigating biological or chemical systems which are consist of particles under different degrees of confinement has got great interest recently. In this work we study a suspensions of disc-like particles between two planar walls by means of simulation. The system under influence of sedimentation along the walls as an external force is considered. The settling speed of a colloid in respect to varying geometrical parameters are calculated. By calculation of velocity profile of the fluid particles, the effect of Hydrodynamic interaction due to solvent's flow in the laminar regime is discussed. In the next step the dependency of the sedimentation velocity on the volume fraction of colloidal particles is considered. Here a hybrid simulation scheme which couples a Molecular dynamic simulation method to a multi-particle-collision (MPC) fluid is used. This is a coarse-grained model to describe fluid dynamics.

CPP 38.14 Wed 17:00 P2

Supramolecular structure changes of tubular J-aggregates on various substrates upon drying from water — •Chien-Lie Lee, Dörthe M. Eisele, Stefan Kirstein, and Jürgen P. Rabe — Humboldt-Universität zu Berlin, Germany

Tubular J-aggregates self-assemble from amphiphilic cyanine dyes in aqueous solution. Although the main driving force for the self assembly results from the hydrophobic effect there are other contributions to the cohesion of the molecules. Therefore, it is possible to transfer these aggregates onto solid substrates where they remain intact, without substantial changes of the morphological and supramolecular structure, as long as as the samples are not completely dried [1].

Here we investigate the role of the hydrophilicity or hydrophobicity of the substrate on the drying and hence destruction of the aggregate structure. The high sensitivity of the optical spectra to changes of the molecular packing within the J-aggregates is used to probe the structure. The hydrophilicity of the substrate is controlled by coating with polyelectrolyte or polymer layers and the drying of the aggregates is recorded time dependent and under controlled humidity.

[1] D.M. Eisele, J. Knoester, S. Kirstein, J.P. Rabe and D.A. Vanden Bout, Nature Nanotech. 4 (2009) 658;

CPP 38.15 Wed 17:00 P2

Self - Assembly of Two Dimensional Ordered Arrays of Mesoscopic Particles on Solid Surfaces — •Züleyha Yenice and Regine von Klitzing — Technische Universität Berlin, Stranski-Laboratorium für Physikalische und Theoretische Chemie, Institut für Chemie, Sekr. TC 9 Straße des 17. Juni 124 D - 10623 Berlin

Self-assembled two-dimensional (2D) colloidal crystals with submicrometer-scale periodicity are of considerable fundamental and technological importance in nanosphere lithography, optical devices, data storage and biosensors as well as model systems for 2D crystallization.

The objective of the current research is to control the distance between particles in a 2D lattice [1]. The deposition of the particles on to the wafer is accruing by spin coating technique. Here the effect of different rotational speed, type of solvent and different concentrations of the particles in the suspension were examined. For morphological observation an atomic force microscope (AFM) operating in the tapping mode was used. However, there is a lack of information about the preparation of high ordered colloidal arrays with the interparticle distance.

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

CPP 38.16 Wed 17:00 P2

Bicontinuous microemulsions at solid surfaces — •Stefan Wellert[1], Ralf Stehle[2], Christoph Schulreich[3], Roland Steitz[2], and Thomas Hellweg[3] — [1]Stranski-Laboratorium für Physikalische und Theoretische Chemie, Inst. f. Chemie TU Berlin, Strasse des 17. Juni 124, D-10623 Berlin — [2]Helmholtz Zentrum Berlin, Hahn-Meitner Platz 1, D-14109 Berlin — [3]Universität Bielefeld, Physikalische und Biophysikalische Chemie (PC III) Universitätsstr. 25, D-33615 Bielefeld

The commercial availability of a large variety of bioinspired surfactants results in a renewed interest in microemulsions being thermodynamically stable self-assembled structures of oil, water and amphiphiles.

Solid surfaces play an essential role in many desired applications. The involved real surfaces can be of variable hydrophobicity due to external influences (e.g. weathering) leading to continuously modified physico-chemical properties of these surfaces. Especially bicontinuous microemulsions are of great interest and the physico-chemical properties of these structure in the bulk phase were studied in many surfactant systems but much less is known about the behaviour or changes of this structure in the presence of a solid surface.

Neutron reflectometry is well suited to resolve the structure of the interface between the microemulsion and the solid surface and we report on measurements on bicontinuous structures on hydrophilic and hydrophobic surfaces. Additionally, we discuss the wetting properties in terms of contact angles at different oil-water ratios at hydrophilic, -phobic and partially hydrophobic surfaces.

CPP 38.17 Wed 17:00 P2

Interactions between geometric defects in 2D colloidal systems — •David Polster, Georg Maret, and Peter Keim — Department of Physics, University of Konstanz, D-78464 Konstanz, Germany

Melting in 2D, according to the Kosterlitz-Thouless-Halperin-Nelson-Young theory, involves the formation and dissociation of topological defect pairs. Because these defects distort the hexagonal symmetric of the 2D crystal it is not possible that an isolated topological point defect is formed. Consequently, topological defects occur always as dislocation or disclination pairs.

Geometric defects on the other hand are isolated point defects which can experimentally created e.g. with an optical tweezer. While topological defects appear already near kT geometric defects need a lot more energy to create. We study the interactions of geometric defects with other defects or the surrounding undisturbed lattice in a 2D system of paramagnetic colloidal particles which are sediment to a water/air-interface. By applying a magnetic field 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. First is created by remove a colloidal particle, second by draw a particle into the crystal.

CPP 38.18 Wed 17:00 P2

Confined Binary Colloidal Crystals in 2D: Monte Carlo Simulation of Crack Formation — •Stefan Medina Hernando, Peter Virnau, and Kurt Binder — Institut für Physik, Uni Mainz, Germany

As recent studies have shown, the confinement of a two-dimensional strip of a binary (A,B) colloidal mixture by walls in one direction may either stabilize or destabilize the crystalline structure depending on the type of wall. However, an introduction of misfit, i.e. a reduction of space between the walls, leads to the appearance of grain boundaries in both cases. These crack patterns typically have a width of several particle diameters and, depending on the extent of the misfit, are spread over the colloidal strip. Large misfits may even drive the system into a glassy state. We also present various methods to characterize order and disorder in such systems.

CPP 38.19 Wed 17:00 P2

Diffusion of amphiphiles and proteins in the bicontinuous phase of a microemulsion: A fluorescence correlation spectroscopy study — •Ralph Neubauer[1], Sebastian Höhn[1], Christoph Schulreich[1], and Thomas Hellweg[2] — [1]Physikalische Chemie I, Universität Bayreuth, Deutschland — [2]Physikalische und Biophysikalische Chemie (PC III), Universität Bielefeld, Deutschland

The bicontinuous phase in a microemulsion is often characterized by dynamic light scattering (DLS) or small angle neutron scattering (SANS). Here we analyze the diffusion of a bicontinuous phase by fluorescence correlation spectroscopy (FCS) to determine the diffusion time and coefficient of tracer particles. FCS is a powerful technique for obtaining readings and results much faster than in an DLS experiment.

In the present work fluorescein labeled amphiphilic molecules are inserted in the microemulsion. By measuring the diffusion of the amphiphiles, the "breathing movement" of the interface layer can be identified. Furthermore, the movement of fluorescent labeled proteins in the water domain is detected and the confinement effect can be identified.

Moreover we compare results from different DLS, SANS and FCS measurements for the bicontinuous phase of sugar surfactant based microemulsions. We also show conclusions for model systems and corresponding systems with technical-grade surfactants. The challenge especially for technical-grade systems is the fluorescence of impurities in the surfactants all over the visible range which cannot be extinguished.

CPP 38.20 Wed 17:00 P2

Crystallization of charged colloids in extreme confinement — •Tetyana Kromer-Vovk, Nadezhda Gribova, and Axel Arnold — ICP, Universität Stuttgart, Germany

Freezing effects in spatially confined fluids and colloidal dispersions receive strong scientific interest over the last decades. Confining surfaces can be found in many contexts like the inner walls of porous materials or in a blood cell. In 3D freezing is a first-order phase transition between liquid and solid phase, while the phase behavior in 2D systems is more complicated since no real long-range translational order exists. The theory predicts a hexatic phase with short-range translational and quasi-long orientational order between liquid and solid. Although several works reported the existence of a hexatic phase in such systems, there still remains debate on the exact nature of the transition.

In our work we present MD simulations of a system of charged colloids in confinement using the ESPResSo software package. We investigated the phase behavior of a two layers system confined between parallel neutral walls. We studied various parameters to check for the presence of a hexatic phase. We find practically no energy barrier to nucleation, clearly showing that the freezing behavior differs from the bulk nucleation scenario. However, instead of an intermediate hexatic phase we find only a region of pronounced crystal-liquid coexistence. We also investigate the influence of various fixed crystal seeds as templates for the crystal phase. The seed enhances the phase separation and through this gives the impression of nucleation around the seed.

CPP 38.21 Wed 17:00 P2

Like-charge attraction in confined colloidal systems — •Dmitriy Rozhkov[1], Sofia Kantorovich[1,2], and Marcello Sega[2] — [1]Ural State University, Lenin av. 51, Ekaterinburg, 620000, Russia — [2]Institute fuer Computerphysik, Universitaet Stuttgart, Pfaffenwaldring 27, 70569, Stuttgart, Deutschland

In Ref. [1] it was shown that DNA molecules in aqueous solution stretched spontaneously along the walls of a glass nanochannel. The attraction of negatively charged spherical colloidal particles to the wedges was also observed. Both effects seem surprising as they demonstrate the attraction of likely charged objects in presence of monovalent salt. At the moment there is no definitive explanation for this effect. Here we use molecular dynamic simulations performed using ESPresSo [2] in order to elucidate the problem using a model system, composed by one colloidal particle and monovalent salt at different concentrations. The results of molecular dynamics simulations are also compared to the solution of the Poisson Boltzmann equation.

[1] M. Krishnan et al, Nano Lett., 7 (5) 1270 (2007) [2] H-J Limbach et al, Comput. Phys. Commun. 174(9) (704-727), 2006

CPP 38.22 Wed 17:00 P2

AFM study on the structuring of silica nanoparticles in confined geometries — •Yan Zeng, Sebastian Schön, and Regine von Klitzing — Stranski-Laboratorium, Department of Chemistry, TU Berlin, Strasse des 17.Juni 124, D-10623 Berlin

Colloidal suspensions are omnipresent in daily life and have many technical applications. To understand the interactions between particles in thin films of colloidal suspensions, we perform force measurements by using Colloidal Probe Atomic Force Microscopy (CP-AFM), in which particles show oscillatory force due to the layer formations of particles under spatial confinement.

Previous works have been done in the field of the effect of particle concentration, particle size and ionic strength on the structuring of the Ludox silica nanoparticles between two rigid confining surfaces. The layer-layer distance in the confined geometry is compared with the mean particle distance from the corresponding free volume case with Small Angle X-Ray Scattering (SAXS).

To understand the effect of confining surfaces properties on the structuring of the nanoparticles in between, confining surfaces are modified thus different surface charge, surface roughness and surface elasticity are obtained. In addition, the adsorption of surfactants on the surface of nanoparticles are studied as well.

CPP 38.23 Wed 17:00 P2

Percolation transition of colloids with short-ranged attraction in a slit-pore geometry. — •Helge Neitsch and Sabine H. L. Klapp — Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

We have performed event-driven molecular dynamic (EDMD) simulations of a system consisting of colloidal particles with ultra-short ranged attractive interactions which are confined by two smooth, parallel walls. The pair-wise interaction between the particles is modeled using a square-well potential with an attraction length of 4% of the particle diameter. In the present system we investigate structural and dynamical properties via quantities like cluster-mass distributions and mean square displacements for the bulk and the confined system using wall distances down to two particle diameters. Above the metastable liquid-liquid spinodal, which has been estimated for the bulk system and all given wall distances, a percolation transition has been found even in the case with the lowest wall distance.

CPP 38.24 Wed 17:00 P2

Exploring the deposition conditions for formation of larger colloidal arrays. — •Matthias Schwartzkopf, Mottakin M. Abul Kashem, Andrew Akbashev, Adeline Buffet, Gerd Herzog, Jessica Lucénius, Jan Perlich, Stephan V. Roth, and Rainer Gehrke — HASYLAB at DESY, Notkestr. 85, D-22603, Hamburg, Germany

Installing regular arrays on mesoscopic length scales plays an important role in nanotechnology. Different techniques of self-assembly via solvent evaporation out of dispersions have been used to obtain highly ordered colloidal structures [Roth]. We used Langmuir-Blodgett (LB) technique and spray deposition [Buffet], representing the most attractive tools for the formation of larger homogeneous colloidal arrays on any kind and shape of substrate. Due to their different deposition and boundary conditions, the assembly behaviour of polystyrene nanoparticles changes, resulting in two-dimensional layers with LB-technique and a large variety of pattern by spray deposition. We present our first results from atomic force microscopy and microbeam grazing incidence small-angle x-ray scattering (*GISAXS).

[Buffet] AEM 2010 accepted

[Roth] APL 2007

CPP 38.25 Wed 17:00 P2

Critical Casimir Forces in Colloidal Suspensions of Janus Particles — •Olga Zvyagolskaya[1] and Clemens Bechinger[1,2] — [1]Universität Stuttgart — [2]Max-Planck-Institut für Metallforschung, Stuttgart

We investigate the behavior of a two-dimensional colloidal system of Janus particles immersed in a critical binary liquid mixture of water and 2,6-lutidine. Janus particles, i.e. particles with antipodal preferential adsorption properties for the two components of the mixture were created by silica particles with a chemical anisotropy. Close to the critical point, critical Casimir forces arise between the particles whose amplitude and sign strongly depend on the temperature and the relative particle orientation. Due to the strong non-isotropic character of these forces, we observe a large variety of colloidal structures in such systems.

CPP 38.26 Wed 17:00 P2

Coupled colloidal particles out of equilibrium — •Carmen Groben[1], Valentin Blickle[1], Jakob Mehl[1], and Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart — [2]Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, 70569 Stuttgart

During the last two decades, there has been considerable progress in the understanding of thermodynamic processes in microscopic systems, where thermal fluctuations cannot be neglected. In this novel field of microscopic thermodynamics, experiments using single colloidal particles play an essential role, since there the phase-space trajectory can be directly observed optically.

To analyse more realistic situations, we extend a well-established single particle technique to study multiparticle nonequilibrium systems. Using rotating laser tweezers, we create two independent nonequilibrium steady states (NESS). Each NESS consists of a single superparamagnetic colloidal particle circulating in a three-dimensional toroidal laser trap. When magnetizing the particles by an external magnetic field, we induce a magnetic dipole-dipole interaction and therefore the coupling between the two NESS becomes adjustable. Depending on the driving forces and the magnetic coupling, we observe large differences in the trajectories of the particles. In our analysis we focus on the effective diffusion coefficient, which exhibits a maximum as a function of the coupling strength.

CPP 38.27 Wed 17:00 P2

The isotope Soret effect in molecular liquids: a quantum effect at room temperatures — •Steffen Hartmann[1], Konstantin Morozov[2], Zina Slimane[1], and Werner Köhler[1] — [1]Physikalisches Institut, Universität Bayreuth — [2]Department of Chemical Engineering, Technion - Israel Institute of Technology, Haifa

In a multicomponent system, a temperature gradient induces a diffusive mass flow, which is counterbalanced in the stationary state by Fickian mass diffusion. The occuring concentration gradient can be described by the Soret coefficient, which can be split into additive contributions. We have developed a theory for the so-called isotopic contribution to the Soret effect of binary liquid mixtures based on the contribution of librational and vibrational motions to the partial pressure. Contrary to its name, the isotopic contribution is not limited to purely isotopic substitution but can be dominating or even sole effect in mixtures of different but chemically similar molecules. To test the theory, we have performed experiments for the binary mixtures from the homologous series of the halobenzenes and for halobenzenes in toluene and cyclohexane, respectively.

CPP 38.28 Wed 17:00 P2

Multicomponent diffusion in microgravity environment — •Matthias Gebhardt, Andreas Königer, and Werner Köhler — Physikalisches Institut, Universität Bayreuth

In particular transport processes in true multicomponent systems ($n > 2$) are still not fully understood and there is a lack of experimental data for ternary and higher mixtures. In many cases the Soret cell, where a liquid sample is placed between two differentially heated copper plates, is used in experiments. The absence of convection is crucial for purely diffusive heat and mass transfer. It is known that many liquids can exhibit negative separation ratios, i.e. heavier components segregate to the hot regions. In gravity fields this has a destabilizing effect on the system and can cause convective instabilities. Microgravity experiments (TRIMIX) are planned using the SODI facility onboard the ISS, which is equipped with a two-color Mach-Zehnder interferometer. We are performing accompanying ground based measurements using a two-color optical beam deflection technique. We provide first experimental results and discuss the influence of the refractive index dispersion relations on the feasibility of the experiments.

CPP 38.29 Wed 17:00 P2

Dispersion study of Carbon Nanotubes — •Gerhard Lackner[1], Viktor Bezugly[2], Daria Kovalenko[3], Anna Czeschik[1], Richard Boucher[2], Jan Meiss[4], and Doru Lupascu[1] — [1]Institut für Materialwissenschaft, Universität Duisburg-Essen, Universitätsstrasse 15, 45141 Essen, Deutschland — [2]Institut für Werkstoffwissenschaft, Technische Universität Dresden, 01069 Dresden, Deutschland — [3]Fraunhofer-Institut für Zerstörungsfreie Prüfverfahren Institutsteil Dresden, IZFP-D, Deutschland — [4]Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden, Deutschland

In this study we focus on the dispersion of carbon nanotubes (CNT) and their characterisation using spectroscopic analysis. Single walled and multi walled carbon nanotubes (SWCNT, MWCNT) are used to form dispersions with different solvents. Besides surface-active agents we investigate a π-stacking approach to disperse the hydrophobic CNT. CNT bucky paper made by DNA-wrapped CNT dispersion include DNA. Covalent sidewall functionalisation of CNT to change their hydrophobic surface to a hydrophilic one will entail additional chains (commonly carboxylic chains) at the CNT sidewall due to the chemical treatment. If surface-active agents are used for preparation, a thoroughly rinsing after film preparation is necessary to remove agents. The π-stacking approach offers the advantage to evaporate all chemicals used for the dispersion via annealing and high purity is achieved. Therefore this technique could be a tool kit in organic semiconducting application.

CPP 38.30 Wed 17:00 P2

Hybrid method simulations of clay suspensions — •Hongliu Yang[1], Martin Hecht[2], and Heike Emmerich[1] — [1]Bayreuth University, Bayreuth, Germany — [2]High Performance Computing Center Stuttgart, Stuttgart, Germany

Clay colloids, in the form of suspensions of platelet particles, are the subject of an enormous recent studies. It is especially due to their widespread applications ranging from drilling, rheology modification for paints, cosmetics, cleansers, and the production of paper, adhesives, synthetic plastics etc. Clay colloid suspensions are different from other colloids by the high anisotropy of the dispersed thin crystalline silicate platelets. Moreover, faces and edges of clay particles may have different types of charges under pH value variation. These factors make the theoretical descriptions of clay suspensions very difficult. A hybrid code with molecular dynamics for clay particles and stochastic rotation dynamics for surrounding fluids is developed by us to simulate clay suspensions. In our simulations clay particles are modeled as charged soft ellipsoids interacting via Gay-Berne potential and screened Coulomb potential. The existence of analytical forms of the mutual interactions makes the calculation of force and torque very efficient. Preliminary results of micro-structures and rheological properties of clay suspensions are reported.

CPP 38.31 Wed 17:00 P2

Weight functions in fundamental measures density functional theory — •Markus Burgis and Matthias Schmidt — Theoretische Physik II, Physikalisches Institut, Universitätsstraße 30, D-95440 Bayreuth

An overview of the key geometrical ingredients of fundamental measures density functional theory is given. In particular the mathematical structure behind the four different types of scalar Kierlik-Rosinberg weight functions is investigated. These weight functions are used to represent the Mayer bond of hard sphere mixtures via pairwise convolution. The range of all weight functions, i.e. the hard sphere radius, can be changed by a convolution transformation. The relevance to both the fundamental measures density functional for additive hard spheres as well as to its generalization to non-additive binary mixtures is discussed.

CPP 38.32 Wed 17:00 P2

IPBS - An iterative Poisson Boltzmann Solver — •Alexander Schlaich — Institute for Computational Physics Universität Stuttgart Pfaffenwaldring 27 70569 Stuttgart

We present a finite element based method for solving the nonlinear Poisson Boltzmann equation in presence of dielectric missmatch with unknown boundary conditions. Such conditions apply for example to colloidal systems with counterions in solution where the field in the inner part of the particle is not of interest.

Proper boundary conditions are determined by an iterative, fast converging procedure which can be applied to arbitrary geometries. This algorithm allows us to solve a wide class of problems, for example in surface chemistry, colloidal science and general soft matter research, with high efficiency due to the reduced number of grid points. Calculation results are compared both to experimental data and theoretical predictions, e.g. those from DLVO theory.

CPP 38.33 Wed 17:00 P2

Entropy and enthalpy convergence of hydrophobic solvation beyond the hard-sphere limit — •Felix Sedlmeier, Dominik Horinek, and Roland Netz — Technical University Munich, Garching, Germany

The experimentally well-known convergence of solvation entropies and enthalpies of different small hydrophobic solutes at universal temperatures seems to indicate that hydrophobic solvation is dominated by universal water features and not so much by solute specifics. The reported convergence of the denaturing entropy of a group of different proteins at roughly the same temperature as hydrophobic solutes was consequently argued to indicate that the denaturing entropy of proteins is dominated by the hydrophobic effect. However, this appealing picture was subsequently questioned since the initially claimed universal convergence of denaturing entropies holds only for a small subset of proteins, for a larger data collection no convergence is seen. We report extensive simulation results for the solvation of small spherical solutes in explicit water with varying solute-water potentials. We show that convergence of solvation properties for solutes of different radii exists but that the convergence temperatures depend sensitively on the solute-water interaction. Accordingly, convergence of solvation properties is only expected for solutes of a homologous series that differ in the number of one species of subunits or solutes that are characterized by similar solute-water interaction potentials. In contrast, for peptides, it means that thermodynamic convergence at a universal temperature can not be expected in general, in agreement with experimental results.

CPP 38.34 Wed 17:00 P2

The Role of Charge Polarization in the Vibrational Dynamics of Ionic Liquids — •Mahdi Taghikhani and Oliver Kühn — Universität Rostock, Institut für Physik, Universitätsplatz 3, D-18051 Rostock

Different theoretical methods for describing the dynamics of the CH-stretching vibrations in imidazolium based ionic liquids ([C2min][NTf2]) are compared. This includes a description in terms of a classical molecular dynamics force field as well as hybrid quantum mechanics/molecular mechanics (QM/MM) approaches with a systematic variation of the partitioning into the QM and the MM parts. Special emphasis is put on the effect of charge polarization on the CH-stretching vibration which is part of a hydrogen bond linking two ions. Equipped with this information a strategy for efficient calculation of linear and nonlinear optical response functions is outlined which is based on the concept of transition frequency correlation functions.

CPP 38.35 Wed 17:00 P2

Bidisperse monolayers: what changes in 2D? — •Elena Minina[1], Alla Dobroserdova[1], Joan Cerda[2], Sofia Kantorovich[1,3], and Christian Holm[3] — [1]Ural State University, Lenin av. 51, Ekaterinburg, 620000, Russia — [2]Institute for Cross-Disciplinary Physics and Complex System, Campus Universitat de les Illes Balears, 07122, Palma de Mallorca — [3]Institute fuer Computerphysik, Universitaet Stuttgart, Pfaffenwaldring 27, 70569, Stuttgart, Deutschland

Ferrofluid microstructure in the absence of an external magnetic field proves to be a function of two main parameters: ferroparticle density and intensity of the magnetic dipole-dipole interparticle interaction. It is also well known, that inherent polydispersity of ferroparticles makes the investigation of the structural transition in ferrofluids even more difficult. Earlier it was proposed to replace a continuous particle size distribution by a model bidisperse one [Ivanov et al, Phys. Rev. E, 2004]. The latter theoretical model provided a very good qualitative agreement on the ferrofluid microstructure with the simulation data [Holm et al, J. Phys: Condense Matter., 2006]. However, direct application of this approach to the description of ferrofluid monolayers (quasi-2D systems of ferroparticles [Klokkenburg et al., Phys. Rev. Lett., 2006]) failed and resulted in the regular qualitative discrepancies with the simulation data. In the present study we modify the free energy functional and show why the interplay of energy and entropy changes significantly ferrofluid microstructure in monolayers.

CPP 38.36 Wed 17:00 P2

Influence of an external magnetic field on a ferrofluid with chain aggregates — •Elena Pyanzina[1], Joan Cerda[2], Sofia Kantorovich[1,3], and Christian Holm[3] — [1]Ural State University, Lenin av. 51, Ekaterinburg, 620000, Russia — [2]Institute for Cross-Disciplinary Physics and Complex System, Campus Universitat de les Illes Balears, 07122, Palma de Mallorca — [3]Institute fuer Computerphysik, Universitaet Stuttgart, Pfaffenwaldring 27, 70569, Stuttgart, Deutschland

We present the analysis of the influence of an external magnetic field on the ferrofluids with intensive interparticle magnetic dipole-dipole interaction. We investigate the structure factor of such systems by means of molecular dynamic simulations and theoretical modeling. In this study we focus on monodisperse systems, i.e. all particles are identical. The theoretical calculations are based on the explicit construction of radial distribution functions from the chain distributions in the presence of an external magnetic field obtained via density functional minimization. Molecular dynamic computer simulation are provided for the verification of the model and for elucidation of the connection between the scattering pattern and the system microstructure.

CPP 38.37 Wed 17:00 P2

Suspensions of particles with shifted magnetic dipoles — •Marco Klinkigt[1], Rudolf Weeber[1], Sofia Kantorovich[1,2], and Christian Holm[1] — [1]University of Stuttgart, Institute for Computational Physics, Pfaffenwaldring 27, 70569 Stuttgar — [2]Ural State University, Lenin av. 57, 620000, Ekaterinburg, Russia

In previous study we investigated the ground state for systems of particles, magnetic moment of which was shifted from the centre of mass, and pointed always outwards radially, using the combination of Monte Carlo simulations and analytical calculations. We showed that antiparallel orientation of moments becomes the most favorable ground state configuration when the shift approaches the particle radius. Our preliminary analysis of relatively small systems at room temperatures also showed a lot of interesting features. To study larger systems we used molecular dynamic simulation to reach better performance. Therefore, we implemented our model in ESPResSo, that allows us to use the P3M algorithm for dipolar long range interactions in systems with periodic boundary conditions in three dimensions. The also implemented MDLC gives us the possibility to simulate monolayers with periodic images in two dimensions. We obtained that the initial slope of the magnetization curves decreases with growing shift parameters. For higher magnetic interaction parameters we find initial slopes lower then the associated Langevin curve. Currently we are carrying out cluster analysis for the systems with different shifts and developing analytical expressions for magnetization laws.

CPP 39: Colloids and Complex Liquids II - Dynamics and Mechanical Properties

Time: Thursday 10:30–13:00 Location: ZEU 222

CPP 39.1 Thu 10:30 ZEU 222

Simplified particulate model for coarse-grained hemodynamics simulations — •Florian Janoschek[1,2], Federico Toschi[1,3], and Jens Harting[1,2] — [1]Eindhoven University of Technology, P.O. Box 513, 5600MB Eindhoven, The Netherlands — [2]University of Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart, Germany — [3]CNR-IAC, Via dei Taurini 19, 00185 Rome, Italy

Human blood flow is a multi-scale problem: in first approximation, blood is a dense suspension of plasma and deformable red cells. Physiological vessel diameters range from about one to thousands of cell radii. Current computational models either involve a homogeneous fluid and cannot track particulate effects or describe a relatively small number of cells with high resolution, but are incapable to reach relevant time and length scales. Our approach is to simplify much further than existing particulate models. We combine well established methods from other areas of physics in order to find the essential ingredients for a minimalist description that still recovers hemorheology. These ingredients are a lattice Boltzmann method describing rigid particle suspensions to account for hydrodynamic long range interactions and—in order to describe the more complex short-range behavior of cells—anisotropic model potentials known from molecular dynamics simulations. Paying detailedness, we achieve an efficient and scalable implementation which is crucial for our ultimate goal: establishing a link between the collective behavior of millions of cells and the macroscopic properties of blood in realistic flow situations. We present our model and demonstrate its applicability to conditions typical for the microvasculature.

CPP 39.2 Thu 10:45 ZEU 222

Structure and Dynamics of AOT Microemulsions with Amphiphilic Diblock Copolymers — •Markus Appel, Robert Wipf, Tinka Spehr, and Bernd Stühn — Institut für Festkörperphysik, TU Darmstadt

We investigate the influence of amphiphilic diblock copolymers on structure and dynamics of the droplet phase of water-in-oil microemulsions based on the surfactant AOT. The size of the droplets is determined by small angle X-Ray scattering experiments, while broadband dielectric spectroscopy (1 Hz to 3 GHz) is used to probe micellar interactions. The temperature-dependent phenomenon of dynamic percolation can be used to estimate the bending modulus of the AOT layer, which is known to be influenced by certain hydrophilic polymers adsorbing to the surfactant layer [1]. Furthermore the dielectric relaxation process in the frequency range $f > 1$ MHz reveals details on droplet-droplet interactions, especially in combination with the static permittivity constant [2].

We are particularly interested in a comparison between simple hydrophilic homopolymers and amphiphilic diblock copolymers in order to study possible 'anchoring effects' of the polymers to the surfactant shell.

[1] R. Wipf et al., Colloid Polym. Sci. (2010) **288**:589-601

[2] D'Angelo et al., Phys. Rev. E (1998) **58**:7657-7663

CPP 39.3 Thu 11:00 ZEU 222

Transient Soret-melting of binary glasses by hot colloids — •Florian Schwaiger and Werner Köhler — Physikalisches Institut, Universität Bayreuth, Germany

Metallic nanoparticles have been investigated for many years in manifold research fields due to their outstanding optical, electronic and thermal properties in soft condensed matter. We have heated gold colloids with a diameter of 250 nm by laser irradiation and used them as microscopic heat sources in a polystyrene/toluene solution. Due to the high absorbance at the plasmon resonance wavelength around 532 nm, significant temperature gradients $\nabla T \propto 1/r^2$ can be achieved in the close vicinity of the particles on length scales below the diffraction limit. As a consequence of the Soret effect, there is a strong nonlinear coupling to the order parameter, the local composition of the binary system. In this binary glass former, a bubble of high mobility due to local toluene enrichment, accompanied by a drastic lowering of the glass transition temperature T_g, is created around the laser-heated particle. Accordingly, the colloidal particle is trapped within a cage of low friction that dynamically forms around the colloid and follows its position with a certain retardation. Outside of this bubble the colloids are virtually immobile.

CPP 39.4 Thu 11:15 ZEU 222

Self-Propelled Thermophoretic Motion of Gold Capped Microparticles — Andreas Bregulla[1], Markus Selmke[1], Ralf Seidel[2], Michael Mertig[3], Klaus Kroy[4], and •Frank Cichos[1] — [1]Molecular Nanophotonics Group, University Leipzig, Linnéstraße 5,04103 Leipzig — [2]DNA Motors Group, BioTeC, University of Technology Dresden, Tatzberg 47-51, 01307 Dresden — [3]Physikalische Chemie, Mess- und Sensortechnik, Technische Universität Dresden,Eisenstuckstr. 5 01069 Dresden — [4]Soft Condensed Matter Theory Group, University Leipzig, Vor dem Hospitaltore 1, 04103 Leipzig

Molecular Motors are the machinery of cells that convert chemical into mechanical energy and transport material in a directed manner. Inspired by these molecular machines a number of different artificial self-propelled swimmers have been realized to mimic the same function for future applications in chip-sized laboratories. Most of these swimmers are, however, based on chemical reactions, which are difficult to control or to interrupt. Here we present the design and function of self-propelled microparticles, which can be addressed and switched externally by a laser field. The self-propelled motion is controlled by optical heating of a thin gold cap on polystyrene particles to generate a temperature gradient. The results on the directed motion of different sized particles provide strong evidence for a thermophoretic driving mechanism. Thus the presented particles provide for the first time a detailed control of the speed of each individual particle.

CPP 39.5 Thu 11:30 ZEU 222

Transport studies of colloidal systems through channels and across barriers — •Christian Kreuter[1], Peter Nielaba[1], Paul Leiderer[1], and Artur Erbe[2] — [1]Universitaet Konstanz — [2]Helmholtz-Zentrum Dresden-Rossendorf

Colloidal particles are ideal model systems for processes on a mesoscopic scale, because the energies, which are determined by the interactions of the particles, are on the same range as the thermal energy provided by the solvent. In these studies we investigate the behavior of superparamagnetic particles, which are driven gravitationally through narrow channels and across lithographically defined barriers. Such systems model many aspects of the behavior of charge carriers in nanoscale conductors. By comparing the experimental results with Brownian dynamics simulations, we can explore a large range of parameters and mimic a large number of known situations. Especially, we find ordering processes, which are induced by the interparticle interactions caused by the magnetic dipole moments of the particles. This leads to a movement of the particles in layers and strongly affects the diffusion behavior of the system.

CPP 39.6 Thu 11:45 ZEU 222

Colloidal particles in multiphase flow — •Florian Günther — TU Eindhoven

Emulsions stabilized by particle 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. In this contribution we present a simulation algorithm based on a multicomponent lattice Boltzmann model to describe the solvents combined with a molecular dynamics solver for the description of the solved particles. In nature colloids are generally not spherical, such as clay particles, which have a platelet like shape. As an example of anisotropic particles we study ellipsoids. Our model allows a wide variation of fluid properties, the aspect ratio m of the ellipsoid and arbitrary contact angles on the particle surfaces. We investigate some features of a single particle at a flat interface between two fluids such as the contact angle depending on particle attributes and the adsorption trajectories. Furthermore, we study the parameter dependence of the model and demonstrate its applicability by studying, at least for the special case of m=1, the formation and rheology of a "bicontinuous interfacially jammed emulsion gel" (bijel) and of a "Pickering emulsion".

CPP 39.7 Thu 12:00 ZEU 222

The effective hydrodynamic radius of single DNA-grafted colloids as measured by fast Brownian motion analysis — •Olaf Ueberschär, Carolin Wagner, Tim Stangner, Christof Gutsche, and Friedrich Kremer — Universität Leipzig

Optical tweezers accomplished with fast position detection enable one to carry out Brownian motion analysis of single DNA-grafted (grafting density: ~1000 molecules per particle, molecular weight: 4000 bp) colloids in media of varying NaCl concentration. By that the effective hydrodynamic radius of the colloid under study is determined and found to be strongly dependent on the conformation of the grafted DNA chains. Our results compare well both with recent measurements of the pair interaction potential between DNA-grafted colloids (Kegler et al. Phys Rev Lett 2008;100:118302) and with microflu-idic studies (Gutsche et al. Microfluid Nanofluid 2006;2:381-386). The observed scaling of the brush height with the ion concentration is in full accord with the theoretical predic-tions by Pincus, Birshtein and Borisov.

CPP 39.8 Thu 12:15 ZEU 222

Force Measuments between colloidal Particles across aqueous electrolytes using CP-AFM — •Liset Luederitz and Regine von Klitzing — Stranski-Laboratorium fuer Physikalische und Theoretische Chemie, Institut fuer Chemie, Technische Universitaet Berlin, Strasse des 17. Juni 124, D-10623 Berlin

The interaction forces between two colloidal silica particles across different electrolytes, CsCl, KCl, NaCl and LiCl were measured using CP-AFM technique. In our study the adsorption of counterions follows the Hofmeister series for CsCl, KCl and NaCl but LiCl has anomalous behaviour. The instability of the hydration shell of lithium could be a reason for the observed anomaly. The DLVO theory explains the interactions between the colloidal particles assuming only two types of forces, repulsive electrostatic forces and attractive van der Waals forces. At short separation some deviations from the theory are reported [1]. These deviations are called non DLVO forces and are present in water and electrolyte solutions. In this work we measured short range attractions at 10^{-4}M ionic strength whereas at 10^{-3}M short range repulsions are observed. Another interesting phenomenon observed was the charge reversal with the studied monovalent ions at 10^{-3}M ionic strength and low pH.

1. Valle-Delgado, J.J.; Molina-Bolivar, J.A.; Galisteo-González, F.; Galvéz-Ruiz, J.; Feiler, A.; Rutland, M.W. J. Chem. Phys. 2005, 123, 12.

Topical Talk CPP 39.9 Thu 12:30 ZEU 222

Combining structure and mechanical properties of colloidal systems — Marcel Roth[1], Chris Grigoriadis[2], Jinyu Zhao[1], Burkhard Mayer[1], Doris Vollmer[1], George Floudas[2], and •Günter. K. Auernhammer[1] — [1]MPI Polymerforschung, 55128 Mainz, Germany — [2]University of Ioannina, 45110 Ioannina, Greece

While observing the sample with confocal microscopy we either determine the mechanical properties with a home-build piezo-rheometer or we submit the sample to electric or magnetic fields. Two examples will be discussed.

In case of PMMA colloids dispersed in the isotropic phase of the liquid crystalline compound 4 cyano-4'-biphenyl (5CB), aggregation is induced by simple cooling through the isotropic-nematic transition. This leads to a complete phase separation of a colloid-free nematic phase and a colloid-rich isotropic phase within a temperature range of (1-2)K, creating a sponge-like network. 5CB is a solvent of PMMA in its isotropic phase and plastificizes PMMA at lower temperatures, as confirmed by rheology [1] and dielectric spectroscopy.

In relatively weak colloidal systems, like colloidal crystals, magnetic probe particles can be used to test the mechanical properties of the system. With the confocal microscope we follow both the motion of the magnetic particles and of the surrounding matrix particles. This allows us correlating the structural changes in the matrix with the mobility of the probe particle.

[1] M. Roth, D'Acunzi, D. Vollmer, and G. K. Auernhammer, J. Chem. Phys. **132**, 124702, (2010).

CPP 40: Polymer Crystallization and Semicrystalline Polymers

Time: Thursday 10:30–13:00 Location: ZEU 160

Topical Talk CPP 40.1 Thu 10:30 ZEU 160

Crystallization in block copolymer thin films — •Christine M. Papadakis[1], Charles Darko[1], and Günter Reiter[2] — [1]TU München, Physikdepartment, Physik weicher Materie, Garching — [2]Universität Freiburg, Fakultät für Physik

Polymer crystallization in microphase-separated block copolymers proceeds in thermodynamic confinement. To characterize the crystalline structure, e.g. the crystal orientation, macroscopic alignment of the domains is required. Numerous experiments have been carried out on bulk samples which were macroscopically oriented by high amplitude shear. The thin film geometry has the advantage that the domains orient macroscopically, and imaging methods can be used to characterize the surface texture of crystallized films. Grazing-incidence X-ray diffraction and small-angle scattering allow a detailed characterization of the crystalline structure in a wide range of length scales.

Two examples will be presented. In thin films of lamellae-forming poly(styrene-b-(ethylene oxide)), we have found that the resulting crystalline structure – the orientation of the chain stems, their orientational distribution and the size of the crystallites – strongly depends on the degree of supercooling. In thin films of cylinder-forming poly(isoprene-b-(ethylene oxide)), crystallization can only proceed very slowly and only at the film surface which is due to a mismatch in crystalline layer thickness and cylinder radius.

CPP 40.2 Thu 11:00 ZEU 160

Growth Pathway and Precursor States in Single Lamellar Crystallization: MD Simulations — •Chuanfu Luo and Jens-Uwe Sommer — Leibniz Institute of Polymer Research Dresden, Dresden, Germany

Molecular dynamics (MD) simulations are carried out to study the growth pathway of a single polymer crystal from a highly entangled dense melt via self-seeding[1]. Linear lateral growth, lamellar thickening and slipping of monomers along the chain direction are directly observed. We have introduced a measure of orientational-temporal persistence to characterize the state of monomer sequences out of equilibrium. This analysis allows us to define a birth-time for each stem and accordingly, folding kinetics of individual chains is analyzed as a function of their lifetime. Two stages can be identified for the growth of stem length with lifetime: The stem length increases linearly with lifetime at the precursor stage while it increases logarithmically at the thickening stage. Folds are created at the precursor stage and refolding events are statistically irrelevant. Precursor states can be identified as an early stage of a stem formed by semi-flexible segments. The semi-flexible segments are possessing orientational-temporal persistence which can potentially crystallize, and can be thus considered as unstable short stems. The classical Lauritzen-Hoffman (LH) or Sadler-Gilmer (SG) models are not consistent with our results which correspond to a time scale of about $\lesssim$ 45 ns. We thank DFG(SO 277/6-1) for financial support and ZIH of TU-Dresden for computing time. [1]C. Luo and J.-U. Sommer, Phys. Rev. Lett. 102, 147801 (2009)

CPP 40.3 Thu 11:15 ZEU 160

Melt dynamics and semi-crystalline structure of polyethyleneoxide — •Albrecht Petzold and Thomas Thurn-Albrecht — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle (Saale)

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

CPP 40.4 Thu 11:30 ZEU 160

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

The effect of alkyl side chain length on the orientation of polymer crystallites was studied for a series of poly(3-alkylthiophene)s (P3ATs) like poly(3-pentylthiophene) (P3PT), poly(3-hexylthiophene), poly(3-heptylthiophene) (P3HeptT), and poly(3-octylthiophene) (P3OT). Thin films were cast on the Si/SiO2 substrate at RT and -30°C. The orientation of the crystallites was studied using x-ray and electron diffraction techniques. The 2D diffraction pattern of -30°C cast P3PT film shows the presence of well in-plane stacked edge-on oriented crystallites which are favor for the charge transport. The scattered intensity of -30°C as-cast films are 5 times higher than the RT cast one and it increase to 8 by treating the substrate with OTS. Surprisingly, the -30°C cast P3OT film has few face-on oriented crystallites. But, the mixed edge- and face-on oriented crystallites were observed in RT cast films and showing the powder like distribution of crystallites. Those face-on oriented crystallite was able to resolve through HRTEM. Such an enhancement in ordering of the crystallites with decreasing the growth temperature and side chain length can be explained by the controlled supersaturation ratio as well as the decrease in flexibility of side chain length which may induce the surface nucleation.

CPP 40.5 Thu 11:45 ZEU 160

Confined dynamics and crystallization in self assembled alkyl nanodomains — •Shireesh Pankaj[1] and Mario Beiner[1,2] — [1]Naturwissenschaftliche Fakultät II, Martin-Luther Universität Halle-Wittenberg, 06099 Halle (Saale), Germany — [2]Fraunhofer-Institut für Werkstoffmechanik, Walter-Hülse-Str. 1, 06120 Halle (Saale), Germany

Long alkyl groups are often used to improve the performance of functional polymers. The methylene sequences in such systems usually show a strong tendency to aggregate to form small alkyl nanodomains which can be either completely amorphous or partly crystalline. The influence of main chain packing, domain size and density on the properties of self-assembled alkyl nanodomains is studied based on a comparison of regio-random and regio-regular poly(3-alkyl thiophenes) (P3ATs) with different side chain length as model systems. We show that the dynamics of the CH2 units in amorphous alkyl nanodomains is mainly independent on the packing and microstructure of the main chains. Relaxation spectra show a similar CH2 dynamics despite of the fact that the thiophene main chains are crystalline in regio-regular but amorphous in the regio-random P3ATs. Reasons for the systematic dependence of the CH2 dynamics on the length of the alkyl groups are considered. The influences of average volume per CH2 unit and geometrical confinement are studied. A competition of main and side chain crystallization mechanisms is discussed which should be considered if higher P3ATs are optimized for optoelectronic applications.

CPP 40.6 Thu 12:00 ZEU 160

Self-assembling in solution of crystalline-amorphous olefin block-copolymers investigated by wide-Q SANS and microscopy — •Aurel Radulescu[1], Günter Goerigk[1], Lewis Fetters[2], and Dieter Richter[3] — [1]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science, 85747 Garching, Germany — [2]School of Chemical and Biomolecular Engineering, Cornell University, Ithaca, New York 14853-5021, USA — [3]Forschungszentrum Jülich GmbH, Institut für Festkörperforschung, 52425 Jülich, Germany

Self-assemblies formed in solution by olefin block-copolymers (OBC) that consist of crystallizable ethylene-octene blocks (hard) with very low co-monomer content and high melting temperature alternating with amorphous ethylene-octene blocks (soft) with high co-monomer content and low glass transition temperature were characterized within a wide temperature range over a wide length scale (between 1nm and 10 μm) by combining optical microscopy with crossed polarizers and pinhole- and mirror-focusing-SANS techniques at the KWS-2 and KWS-3 small- and very-small-angle diffractometers set up at the FRM II reactor in Garching. Complex aggregates revealing multiple size levels and hierarchical structural organization were fully characterized with respect to the morphology and the geometrical and density parameters.

CPP 40.7 Thu 12:15 ZEU 160

Application of Optical Coherence Tomography (OCT) for Monitoring the Crystallization of Polymers — •Peter Hierzenberger[1], Gerhard Eder[1], Elisabeth Leiss-Holzinger[2], and David Stifter[1] — [1]Johannes Kepler University, Linz, Austria — [2]Research Center for Non Destructive Testing GmbH, Linz, Austria

The use of Optical Coherence Tomography (OCT) as a novel non-destructive method for the investigation of structure development during polymer solidification is demonstrated. It is well known that the application of high shear gradients to crystallizable polymers produces highly oriented structures, whose development can be monitored by measuring the increasing optical retardation of the transmitted light. However, the increasing turbidity limits this method to conditions far from processing. By use of OCT - which measures reflected light in an interferometer arrangement - we are now able to go directly into that range and extend the experimental window to conditions more relevant to industrial polymer processing.

As a typical schedule molten isotactic poly(propylene) is extruded through a slit die, then quenched to a temperature slightly below the melting point, and after thermal equilibration sheared by resuming extrusion for a certain time. OCT enables on-line observation of structure development and gives depth-resolved images, which can be evaluated quantitatively afterwards and show the growth of the birefringent structures. Additionally, the cooled sample can be extracted and analyzed under the polarization microscope. Comparison of those ex-situ images with in-situ OCT images serves as validation of the method.

CPP 40.8 Thu 12:30 ZEU 160

How Do Extended Chain Crystals Affect the Surface Morphology of Diblock Copolymers? — •Thomas F. Keller, Stefan Watzke, Robert Schulze, and Klaus D. Jandt — Institute of Materials Science and Technology (IMT), Friedrich-Schiller-University Jena, Germany

Recently, in short chain double-crystalline diblock copolymers several temperature-dependent morphologies were reported, which are suppressed in similar high molecular weight copolymers. These morphologies were attributed to extended chain crystals with enhanced chain mobility at the interfacial boundary to neighboring domains.

The aim of the presented study was to test the hypothesis that these temperature-dependent morphologies form on the surface of thin films of such copolymers, and to investigate the phase separation as well as the nucleation and crystal growth behaviour.

By in-situ atomic force microscopy (AFM) we analyzed the temperature-dependent surface morphology of thin films of a short chain polyethylene-block-poly(ethylene oxide) copolymer. When cooling from the melt we observed a heterogeneous surface morphology. Needle-like plates formed. In between these needle-like plates a perpendicular lamellar morphology gradually built up.

A model to describe these observations is discussed, which bases on the formation of extended chain crystals. The current study shows how this formation of extended chain crystal induces new heterogeneous nanostructured copolymer surfaces for potential applications, such as in the biomedical field.

CPP 40.9 Thu 12:45 ZEU 160

Single Molecule Studies of Stress Relaxation in Elastomeric Polyproplyene — •Stefan Krause[1], Martin Neumann[2], Melanie Bibrach[2], Harald Graaf[1], Robert Magerle[2] und Christian von Borczyskowski[1] — [1]Center for Nanostructured Materials and Analysis, Chemnitz University of Technology D-09107 Chemnitz, Germany — [2]Chemische Physik, Chemnitz University of Technology

Since the early 90s, single molecule (SM) spectroscopy studies provided a manifold of new information about systems with heterogeneities, such as biological systems, polymer melts and glasses. The fluorescence of a SM is a very sensitive probe and changes of the fluorescence lifetime, the emission wavelength, and the polarization can report spatial and temporal variations in the environment with high sensitivity[1]. Here we report on SM microscopy and spectroscopy studies of stress relaxation in thin films of elastomeric polypropylene, a semicrystalline polymer with a complex microstructure of crystalline and amorphous regions on the nanometer scale. The films are strained in-situ using a microtensile testing setup and the temporal evolution of mechanical stress is measured. Simultaneously, perylenediimide dyes embedded in the ePP film as isolated dye molecules or covalently linked to ePP molecules report their molecular dynamics and changes within their local environment via SM spectroscopy. This experiment allows for insights into the molecular dynamics within the amorphous regions of ePP which are not accessible with other microscopy techniques.

[1] S. Krause, P. F. Aramendia, D. Täuber and C. von Borczyskowski, 2011, PCCP, accepted.

CPP 41: Glasses and Glass Transition II (jointly with DY, DF)

Time: Thursday 10:45–13:00 Location: ZEU 114

Topical Talk CPP 41.1 Thu 10:45 ZEU 114

Local Anisotropy of Fluids, Glasses and Jammed Bead Packs — •Gerd Schroeder-Turk — Theoretische Physik, Friedrich-Alexander Universität Erlangen-Nürnberg, Staudtstr 7B, 91058 Erlangen

The local structure of particle ensembles is important for physical properties of normal or super-cooled fluids, jammed bead packs or structural glass phases. It is often characterized by order parameters such as q_4 or q_6, defined by spherical harmonics of particle neighborhoods. Here we show that a Minkowski tensor analysis of the particles' Voronoi cells provides shape indices that give a clear signature of various structural transitions in particle systems. In particular, all of the above mentioned systems consist of locally anisotropic environments. We show that the degree of cell anisotropy shows a clear signature of the jamming transition in bead packs, the transition to partially ordered states at the random close packing limit, and of the transitions from fluid to ordered phases in simple liquids. For jammed bead packs, these findings suggest an inherent geometrical reason why anisotropic shapes can fill space more efficiently than spheres.

[1] Schröder-Turk *et al*, Europhys. Lett., **90**(3), 34001 (2010)
[2] Kapfer *et al*, J. Stat. Mech. (2010) P11010

CPP 41.2 Thu 11:15 ZEU 114

In-situ characterization of vapor-deposited glasses of toluene by differential AC chip nanocalorimetry — •Mathias Ahrenberg[2], Heiko Huth[2], Katie Whitaker[1], Mark D. Ediger[1], and Christoph Schick[2] — [1]University of Wisconsin - Madison — [2]University of Rostock

We use ac nanocalorimetry to investigate extraordinarily stable glasses of toluene prepared by vapor deposition. For that purpose we have built a vapor deposition chamber that allows in-situ characterization of vapor-deposited organic glasses down to liquid nitrogen temperature. With highly sensitive nanocalorimeters in a differential setup, we are able to measure ng-samples over a frequency range from 0.1 Hz up to 8 kHz. The device was used to investigate the transformation of as-deposited stable toluene glasses into ordinary glasses. For films about 100 nm thick, the transformation was studied as a function of time at constant temperature above the common glass transition and as function of temperature at constant heating rate. The stability of the thin films was investigated as a function of substrate temperature and deposition rate.

CPP 41.3 Thu 11:30 ZEU 114

Structural relaxation times in high-density amorphous ice (HDA) — •Philip H. Handle[1], Markus Seidl[1], Erwin Mayer[2], and Thomas Loerting[1] — [1]Institute of Physical Chemistry, University of Innsbruck, Austria — [2]Institute of General, Inorganic & Theoretical Chemistry, University of Innsbruck, Austria

Solid water (H2O) exists in a variety of different forms. Besides common hexagonal Ice (Ih) today 15 different crystalline and three different amorphous forms are known. It is under discussion whether the amorphous forms are glassy (related to liquid water [1]) or nano-crystalline (related to ice). In case of high-density amorphous ice (HDA) this question has been addressed in some studies [2-4], yet remains controversial. In our work we measured structural relaxation times of HDA at elevated pressures (0.1 and 0.2 GPa) and different temperatures (125-135 K) on the basis of differential scanning calorimetry (DSC) at 1 bar. Our data suggest that at 135 K the structural relaxation time is only slightly higher than 100s, i.e., HDA is on the borderline to the glass transition.

[1] Poole, P. H.; et al.; Nature 360, 324-328 (1992). [2] Tse, J. S.; et al.; Nature 400, 647-649 (1999). [3] Mishima, O.; J. Chem. Phys. 115, 4199-4202 (2001). [4] Andersson, O.; Phys. Rev. Lett. 95, 205503-205507 (2005).

CPP 41.4 Thu 11:45 ZEU 114

Dynamics of glass forming liquids in soft confinement — •Emmanuel Gouirand[1], Thomas Blochowicz[1], Andreas Blank[1], Bernd Stühn[1], and Bernhard Frick[2] — [1]Institut für Festkörperphysik, TU Darmstadt — [2]Institut Laue-Langevin, Grenoble, France

In search of a characteristic length scale associated with cooperative dynamics at the glass transition, intensive effort has been devoted to investigating the influence of confinement on the dynamics of glass forming liquids. Nevertheless, no generally accepted picture exists so far because of the complex interplay of surface, pressure and finite size effects affecting the dynamics. We investigate the dynamics in confinements of different nature in order to be able to disentangle these various effects. Therefore, we apply photon correlation spectroscopy and quasi elastic neutron scattering on glass formers confined within microemulsion droplets, the structure of which proved to remain stable over the whole temperature range by means of small angle scattering. First, we report on the dynamics of glycerol confined in AOT micelles where the glass transition temperature (T_g) of the matrix is chosen to be smaller than T_g of the glycerol core (fast soft confinement). We find glycerol to relax faster than in bulk with an Arrhenius temperature dependence [1]. Then we compare the dynamics of toluene in Cremophor ELP micelles. Contrary to the former situation, here the matrix relaxes slower than the core and slows down the latter due to interfacial effects. Finally, below T_g of the matrix actual hard confinement of toluene within the droplets is realized.
[1] Blochowicz et al., CPL 475, 171-174 (2009)

CPP 41.5 Thu 12:00 ZEU 114

Crystallization and induced glass transition of n-alcohols in silicon-nanochannels — •Rolf Pelster, Rene Berwanger, Carsten Biehl, and Christoph Schuhmacher — FR 7.2 Experimentalphysik, Universität des Saarlandes, D-66123 Saarbrücken, Germany

We have investigated the molecular dynamics of n-alcohols (C_4H_9OH - $C_{11}H_{23}OH$) confined in mesoporous silicon and silicon oxide with pore radii ranging from 3.5 to 7 nm. Using dielectric and infrared spectroscopy we show that the temperature of the liquid-solid phase transition and the structure of the solid phase depend on both the chain length and the radius of the pores:

Long-chain alcohols exhibit a crystalline structure at low temperatures. The confinement induces a lowering of the freezing temperature. The shorter the chain length or the smaller the pore radius, the lower the freezing temperature. Below the phase transition only the dynamics of amorphous wall layers are observable [1].

Short-chain alcohols behave differently. While bulk alcohols still freeze upon slow cooling, we observe a glass transition for the confined phase. The glass transition temperature is close to that reported for quenched bulk alcohols. We thus conclude that nano-confinement suppresses the crystallization process and induces a glass transition.

[1] R. Berwanger, Ch. Schumacher, P. Huber, and R. Pelster, Eur. Phys. J. Special Topics 189, 239-249 (2010)

CPP 41.6 Thu 12:15 ZEU 114

Glass Transition in Confined Geometry — •Simon Lang[1,2], Viatlie Botan[1], Martin Oettel[1], David Hajnal[1], Thomas Franosch[2], and Rolf Schilling[1] — [1]Johannes Gutenberg-Universität Mainz, Germany — [2]Universität Erlangen/Nürnberg, Germany

Confinement of a simple liquid is accompanied by introducing a further length scale in addition to the average distance of the particles. The interplay between them strongly influences the glass transition according to numerous significant experiments and simulations.

To achieve a theoretical description, we extend the microscopic mode-coupling theory to a liquid confined between two parallel flat hard walls [1]. The theory contains the standard mode-coupling equations in bulk and in two dimensions as limiting cases and requires as input solely the equilibrium density profile and the static structure factors of the fluid in confinement. We evaluate the phase diagram for a hard-sphere liquid as a function of the distance of the plates and obtain an oscillatory behavior of the glass transition line as a result of the structural changes related to layering. We detect a facilitation of the glass transition at half-integer values of the distance with respect to the hard-sphere diameter. In contrast, at commensurate packing particles can more easily slide along the walls and therefore the liquid phase remains favored for higher packing fractions.
[1] S. Lang, V. Botan, M. Oettel, D. Hajnal, T. Franosch, and R. Schilling, Phys. Rev. Lett. 105 125701 (2010)

Topical Talk CPP 41.7 Thu 12:30 ZEU 114

Concentration fluctuations and intrinsic confinement effects in binary glass forming liquids: Insights from neutron scattering and X-ray photon correlation spectroscopy — •Thomas Blochowicz[1], Sebastian Schramm[1], Emmanuel Gouirand[1], Philipp Gutfreund[2], Bernd Stühn[1], Bernhard Frick[2], and Yuriy Chushkin[3] — [1]TU-Darmstadt, Darmstadt, Germany — [2]ILL, Grenoble, France — [3]ESRF, Grenoble, France

We investigate the dynamics in a series of binary glass forming liquids using dielectric spectroscopy (DS) in combination with quasielastic neutron scattering, dynamic light scattering and X-ray photon correlation spectroscopy (XPCS). It turns out that, although macroscopically the systems are fully miscible in the whole temperature range, two glass transitions can be clearly distinguished due to the high T_g contrast of the components. By means of DS the corresponding relaxation processes are identified, and it turns out that contrary to expectation the small molecules take part in both glass transitions, which suggests that two dynamical species can be distinguished among the small molecules. Moreover, the relaxation connected with the lower glass transition shows properties typical of dynamics in confinement like an Arrhenius-type temperature dependence and a broad distribution of relaxation times. On the other hand it is revealed by XPCS that the concentration fluctuations exhibit a significantly weaker temperature dependence than the α-relaxation and show a crossover from a diffusive to a so-called ballistic wave vector dependence and from stretched to compressed relaxation functions around the upper T_g.

CPP 42: Transport and Spectroscopy in Molecular Nanostructures II (related to SYMN, jointly with CPP)

Time: Thursday 10:30–13:00 Location: TOE 317

CPP 42.1 Thu 10:30 TOE 317

Ultrafast electronic dynamics in a polyfluorene based guest-host system — •Henning Marciniak, Maik Teicher, and Stefan Lochbrunner — Institut für Physik, Universität Rostock

Guest-host systems are frequently used for organic solid state lasers to achieve tunability of the emission wavelength and low lasing thresholds. Efficient excitation energy transfer from the host to the guest material and the behavior at high exciton densities are thereby important. We investigate a polyfluorene based guest-host system that shows optically pumped lasing in a distributed feedback structure [1]. Combined analysis of steady state and time resolved spectroscopic studies gives rise to a complex picture of the photoinduced dynamics. Steady state and time resolved fluorescence measurements on the nanosecond timescale show emission signatures from the guest material pointing to efficient excitation transfer from the hostto the guest. However, femtosecond pump probe absorption measurements find no signatures of stimulated emission from the guest material but pronounced nonlinear dynamics on the picoseconds timescale. As one quenching mechanism amplified spontaneous emission from the host system is identified, which arises under high excitation densities. However, since the excitation parameters are similar to the nanosecond fluorescence measurements, additional mechanisms have to be taken into account.

[1] T. Riedl, T. Rabe, H.-H. Johannes, W. Kowalsky, J. Wang, T. Weimann, P. Hinze, B. Nehls, T. Farrell, and U. Scherf, *Appl. Phys. Lett.* **88** (2006), 241116.

CPP 42.2 Thu 10:45 TOE 317

Molecular aggregates: handling a complicated vibrational quasi-continuum with non-Markovian quantum state diffusion — •Gerhard Ritschel, Jan Roden, and Alexander Eisfeld — MPI-PKS Dresden

The electronic excitation transfer and the optical processes in molecular aggregates, e.g. light harvesting systems or H-aggregates, are strongly influenced by the coupling to vibrational degrees of freedom – these are internal vibrational modes of the monomers as well as vibrations of the environment. For an adequate theoretical description, that allows us to understand the dynamics of these systems, it is therefore essential to include the vibrations in the calculations.

To this end we apply a new approach, that is based on a non-Markovian quantum state diffusion treatment: a time-dependent stochastic Schrödinger equation for an electronic wave function is solved numerically and the reduced density operator is obtained by averaging over many realizations of the stochastic noise.

This efficient method enables us to calculate spectra and energy transfer dynamics in a non-perturbative way. It is now possible to capture the whole range from coherent dynamics to incoherent diffusion and to investigate the influence of a complicated structured quasi-continuum of vibrations.

Phys. Rev. Lett. **103**, 058301 (2009)

CPP 42.3 Thu 11:00 TOE 317

Time-resolved electron-transfer properties of a low-band-gap neutral mixed-valence polymer — •Florian Kanal[1], Tatjana Quast[1], Martin Kullmann[1], Stefan Ruetzel[1], Johannes Buback[1], Sabine Keiber[1], Dörte Reitzenstein[2], Christoph Lambert[2], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg — [2]Institut für Organische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg

We present measurements of the electron-transfer properties of a polyradical consisting of alternating triarylamine donor and triarylmethyl radical acceptor moieties. This first polymeric neutral mixed-valence compound is attractive for applications due to its low band gap. It shows an intervalence charge transfer (IVCT) band in the near infrared. The polyradical and a reference monomer were investigated by liquid-phase fs pump–probe spectroscopy in two different solvents. Excited in the visible spectral range and probed with a whitelight supercontinuum, the transient spectra of the polyradical feature two bands around 550 nm and 650 nm. These bands are assigned to characteristic transitions of the anion and the radical cation, respectively, formed upon optically induced electron transfer. The decay curves exhibit a biexponential decay in the ps time regime. The short-living – solvent dependent – component refers to the direct decay from the IVCT state to the ground state. The long-living – solvent independent – component is tentatively attributed to an equilibrium formation of the IVCT state and a completely charge-separated state.

CPP 42.4 Thu 11:15 TOE 317

Electronic properties of semiconducting polymer nanotubes — •Thomas Plocke[1], Matthias Müller[1], Janina Maultzsch[1], Christian Thomsen[1], Andreas Stefopoulos[2], Souzana Kourkouli[3], Elina Siokou[3], Kostas Papagelis[3], and Joannis Kallitsis[2,3] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Foundation for Research and Technology Hellas, Institute of Chemical Engineering and High Temperature Processes (FORTH-ICEHT), 26504, Patras, Greece — [3]University of Patras, 26504, Patras, Greece

Single-walled carbon nanotubes were functionalized with different polymeric quinoline chains using the ”‘grafting from”’ approach in order to combine the properties of the semiconducting polymers with those of the carbon nanotubes [1]. We perform a resonant Raman spectroscopy analysis to study the influence of the functionalization on the electronic properties and the optical transitions of the modified tubes. We observe that the electronic properties of the nanotube derivatives change due to doping effects caused by charge transfer between the tubes and the polymers. Interestingly, our results on different functionalized single-walled carbon nanotubes show frequency shifts for the Raman G-mode in both directions compared to the pristine material. The preparation pathway of the studied samples allows us to distinguish structural from electronic effects caused by the polymer and the metal ion.[1] A. A. Stefopoulos, S. N. Kourkouli, E. Siokou, K. Papagelis, M. Müller, T. Plocke, J. Maultzsch, C. Thomsen, J. K. Kallitsis; in preparation (2010).

CPP 42.5 Thu 11:30 TOE 317

Conductance enhancement of InAs/InP heterostructure nanowires by surface assembly of oligo-phenylenevinylene molecular wires — •Muhammed Ihab Schukfeh[1], Kristian Storm[2], Roar Søndergaard[3], Anna Szwajca[1], Allan Hansen[1], Peter Hinze[4], Thomas Weimann[4], Claes Thelander[2], Frederik

C. Krebs[3], Lars Samuelson[2], and Marc Tornow[1] — [1]Institut für Halbleitertechnik, TU Braunschweig — [2]Lund University, Solid State Physics, Sweden — [3]Risø DTU, Technical University of Denmark — [4]PTB, Braunschweig

The direct combination of organic molecules with semiconductor nanostructures provides an appealing approach towards possible future nanoelectronic systems. In this context, indium-arsenide is a material of particular interest due to the presence of an electron inversion layer at the surface. We have prepared 50 nm diameter InAs nanowires comprising a 5 nm long InP segment, and contacted them by Ti/Au metallic leads on a planar Si/Si-oxide substrate. Electronic transport measurements at 77 K confirmed the presence of the potential barrier of the InP segment. After investigation of the assembly of 12 nm long, dithiolated oligo-phenylenevinylene (OPV) derivative molecules from solution onto planar InAs surfaces the same recipe was applied to the InAs/InP nanowires, which led to a pronounced, non-linear I-V characteristic, with significantly increased currents of up to 1 μA at 1 V bias, for a back-gate voltage of 3 V. We attribute this effect to the OPV molecules tethered to the nanowire surface, thereby increasing the surface conductance across the InP barrier.

CPP 42.6 Thu 11:45 TOE 317

Modeling the blinking dynamics of single CdSe/ZnS quantum dots probing their local environment — •Cornelius Krasselt[1], Robert Schmidt[1], Jörg Schuster[1,2], and Christian von Borczyskowski[1] — [1]Institute of Physics and nanoMA (Center for nanostructured Materials and Analytics), Chemnitz University of Technology, Germany — [2]now: Fraunhofer Institute ENAS

Fluorescence intermittency, also known as blinking, appears to be a common feature of many different classes of individual emitters like semiconductor quantum dots. Generally it is characterized by inverse power law distributions for both the on- and off- times [1] which are due to trapping and detrapping processes of charges in- and outside the quantum dots, respectively.

This contribution discloses the influences of the local environment surrounding ZnS coated CdSe quantum dots on silicon oxide on their blinking dynamics. We present atypical distributions for the on-time statistics which show deviations from the expected power law behaviour only seen at the beginning of the statistics. These deviations correlate to the local density of hydroxyl groups on silicon oxide but are also measured in polymers such as PS and PVA. Furthermore we are able to resolve the intensity levels of quantum dot time traces via intensity-changepoint analysis observing an increasing density of bright intensity levels in case of enhancing on-time deviations accompanied by longer exciton lifetimes. All results are discussed in terms of a model concerning hole trapping processes within the quantum dots.

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

CPP 42.7 Thu 12:00 TOE 317

Off-time distribution in blinking quantum dots: theoretical investigation — •Peter Reineker[1], Thomas Hartmann[1], and Vladimir Yudson[1,2] — [1]Institute of Theoretical Physics, Ulm University, Albert-Einstein-Allee 11, 89069 Ulm, Germany — [2]Institute for Spectroscopy, Russian Academy of Sciences, Troitsk, Moscow region, 142190, Russia

The understanding of blinking quantum dots (QDs) is an open problem since more than a decade. We have investigated the off-time distribution of a semiconductor QD on the basis of an Auger-induced release process of an electron deeply trapped in the QD shell. This release process has not yet been treated in the literature explicitly and starts with the optical generation of an additional electron-hole pair in the off-state of a QD, characterized by a valence band hole in the core and a trapped electron in the shell. This additional pair subsequently recombines and the recombination energy is transferred by an Auger process to the trapped electron. We discuss the efficiency of the release process as compared to the quenching process. For a deep trap occupation density $\sim 1/r_0^6$ (r_0 is the trap distance from the QD center) and a Förster-like release rate, we arrive at an off-time distribution $\sim 1/t_{off}^{\alpha}$ with $\alpha = 3/2$ in agreement with experimental findings in many QDs.

CPP 42.8 Thu 12:15 TOE 317

Novel Multi-Chromophor Light Absorber Concepts for DSSCs for Efficient Electron Injection — •Robert Schütz[1], Christian Strothkaemper[1], Carlo Fasting[2], Inara Thomas[1,2], Andreas Bartelt[1], Thomas Hannappel[1], and Rainer Eichberger[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Institut für Organische Chemie, Freie Universität Berlin, Takustraße 3, 14195 Berlin, Germany

Dye sensitized solar cells (DSSCs) operate by injecting electrons from the excited state of a light-harvesting dye into the continuum of conduction band states of a wide bandgap semiconductor. The light harvesting efficiency of pure organic dyes is limited by a narrow spectral electronic transition. A beneficial broad ground state absorption in the VIS region can be achieved by applying a single molecular dye system with multiple chromophors involving a Förster resonance energy transfer (FRET) mechanism for an efficient electron injection. A model donor acceptor dye system capable for FRET chemically linked to colloidal TiO_2 and ZnO nanorod surfaces was investigated in UHV environment. We used VIS/NIR femtosecond transient absorption spectroscopy and optical pump terahertz probe spectroscopy to study the charge injection dynamics of the antenna system. Different chromophors attached to a novel scaffold/anchor system connecting the organic absorber unit to the metal oxide semiconductor were probed.

CPP 42.9 Thu 12:30 TOE 317

Single molecule diffusion in columnar functionalized mesoporous rods — •Florian Feil, Valentina Cauda, Jens Michaelis, Thomas Bein, and Christoph Bräuchle — Physikalische Chemie, LMU München, Germany

Mesoporous silica materials are ideally suited as host-guest systems in nanoscience with applications ranging from molecular sieves, catalysts, nanosensors to drug delivery systems. For all these applications a thorough understanding of the interactions between the mesoporous host system and the guest molecules is vital. Here, we investigated fluorescent dyes as guest molecules acting as molecular probes that were loaded into the channels of mesoporous filaments. The dye AS-TDI was used as a tool to explore the nanoporous channel structure. By sputtering the sample with a very thin layer of gold, which quenches all molecules on the surface, we could show that the molecules were diffusing inside the structure along the columnar channels. Additionally, we could measure the orientation of the TDI molecules, as the channels have such a small diameter that the molecules are not able to rotate freely but have to align parallel to the channels. In a further approach we also succeeded in loading fluorescently labelled DNA into such a mesoporous host system. As mentioned above, we ensured by gold-sputtering that the DNA resides inside the channels and not on the surface of the filaments. Finally, it could be shown by using FRET measurements that the DNA is still intact inside the mesopores. Moreover, we were able to observe DNA diffusion inside the filament channels.

CPP 42.10 Thu 12:45 TOE 317

Characterization of non-covalently modified carbon nanotubes by Raman spectroscopy — •Daria Kovalenko[1,2], Anindya Majumder[2], and Jörg Opitz[1,2] — [1]Fraunhofer Institute for Non-Destructive Testing, 01109 Dresden — [2]Institute for material science, Dresden University of technology, 01062 Dresden

Raman spectroscopy is a technique which allows getting information about chemical structure of the molecules. Recently it got widely used for examinations of carbon based materials. In this study Raman and UV/VIS spectroscopic techniques were used to characterize the process of modification of carbon nanotubes. Single walled carbon nanotubes were non-covalently bounded using different surfactants. By UV/VIS spectroscopy it was established what surfactants react better with the nanotubes and therefore they become more soluble in water. Raman spectra of the dispersions were obtained. Using them, we got information about the structure of the carbon nanotubes. By the wavenumber of RBM-modes in spectra of the CNT dispersions diameter of the nanotubes were calculated and possible chiralities were proposed. By comparing G- and D-band intensities presence and amount of semiconducting and metallic carbon nanotubes were determined.

CPP 43: Nanoparticles and Composite Materials I

Time: Thursday 14:00–18:30 Location: ZEU 222

Topical Talk CPP 43.1 Thu 14:00 ZEU 222

NanoModel - Multi-Scale Modelling of Nano-Structured Polymeric Materials — •Horst Weiss — Polymer Research , BASF SE

The practice of adding micron sized inorganic filler particles to reinforce polymeric materials can be traced back to the early years of the composite industry. With synthetic methods that can produce nanometer sized fillers, resulting in an enormous increase of surface area, polymers reinforced with nanoscale particles should show vastly improved properties. Yet, experimental evidence suggests that a simple extrapolation of the design paradigms of conventional composites cannot be used to predict the behavior of nanocomposites. The origin of these differences between conventional and nanocomposites is still unknown. This, unfortunately, precludes yet any rational design. Though some property improvements have been achieved in nanocomposites, nanoparticle dispersion is difficult to control, with both thermodynamic and kinetic processes playing significant roles. This talk reports on the progress made in a European project called NanoModel. The goal of this project is to develop, implement and validate multiscale methods to compute the mechanical, thermochemical and flow behavior of nano-filled polymeric materials * based on the chemistry-of selected model systems.

CPP 43.2 Thu 14:30 ZEU 222

Modelling of stress and strain amplification effects in filled polymer melts — •Jan Domurath, Marina Saphiannikova, and Gert Heinrich — Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Strasse 6, 01069 Dresden

When hard filler particles are added to a polymer melt, it is usually assumed that it's zero-shear viscosity and therefore the stress increase according to Einstein's or a similar formula. In some papers one finds an alternative approach in which the local strain field is increased according to these formulas. Although both approaches provide the same increase of the shear stress in the linear limit, it can be shown that the second approach violates the energy conservation law as the macroscopic and microscopic dissipated energies are not equal anymore. In this contribution we propose a new stress and strain amplification approach in which both the stress and strain tensors are modified to describe the behaviour of filled polymer melts in the non-linear shearing regime. The new approach is tested using relatively simple constitutive models for description of nonlinear viscoelastic behaviour in polymer melts. The stress and strain amplification approach enables us to explain the peculiar behaviour of the overshoot peak observed recently in filled LDPE melts [1].

[1] F.R. Costa et al. Adv. Polym. Sci. 210, 101 (2008)

CPP 43.3 Thu 14:45 ZEU 222

Structure Property Relationships of Nanocomposites based on Polypropylene and Layered Double Hydroxide — •Purv Purohit, Jesus Sanchez, and Andreas Schönhals — BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany

Nanocomposites based on Polypropylene (PP) and modified ZnAl Layered Double Hydroxides (ZnAl-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. Space resolved SAXS investigation show that the samples are homogeneous on a length scale of several cm and have a predominantly exfoliated morphology. DSC and WAXS show that the degree of crystallinity decreases with the increasing content of LDH. The extrapolation of this dependence to zero estimates a limiting concentration of c.a. 40% LDH where the crystallization of PP is completely suppressed. 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 dodecylbenzene sulfonate (SDBS), which are adsorbed at the LDH layers. Therefore, analysis of the beta-relaxation provides information about the interfacial region between the LDH layers and the PP matrix. The glass transition temperature in this interfacial region is by 30 K lower than that of PP. This is accompanied by a change of the fragility deduced from the relaxation map.

CPP 43.4 Thu 15:00 ZEU 222

Small-angle scattering study of dispersion ability of polystyrene modified carbon nanotubes. — •Anastasia Golosova[1,2], Joseph Adelsberger[1], Alessandro Sepe[1], Martin Niedermeier[1], Sergio S. Funari[3], Peter Lindner[4], Rainer Jordan[2], and Christine M. Papadakis[1] — [1]TU München, Physikdepartment, Fachgebiet Physik der weichen Materie, Garching — [2]TU München, Department Chemie, Lehrstuhl für Makromolekulare Chemie, Garching — [3]HASYLAB at DESY, Hamburg — [4]ILL, Grenoble, France

Carbon nanotubes (CNTs) are attractive for nanocomposite applications due to their unique physical properties. In order to optimize their use as fillers, thorough characterization of their dispersions is of importance. Using small-angle scattering, we have studied the effect of the level of the CNTs' modification with polystyrene grafts on both, the morphology of CNTs and their agglomeration behavior in toluene dispersions. By contrast matching with the solvent in neutron experiments, we highlighted the polymer shell or the CNTs themselves, whereas X-rays gave overall information. The structure of the CNTs and their agglomerates were modeled as fractal aggregates of rods or of core-shell cylinders. The models were found to be consistent with the results of AFM and thermo-gravimetric analysis. Though agglomeration is observed even for the modified CNTs, an increase of the mesh size in the agglomerates with the increase of the modification level indicates that the modification procedure indeed leads to an improved dispersion ability of the CNTs.

CPP 43.5 Thu 15:15 ZEU 222

Experimental study of the structure of aligned CNT/PS composites — •Marina Khaneft[1], Bernd Stühn[1], Jörg Engstler[2], Jörg Schneider[2], and Tinka Spehr[1] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt — [2]Eduard Zintl-Institute für Anorganische und Physikalische Chemie, Technische Universität Darmstadt

We present experimental studies of the infiltration of polystyrene (PS) into the free interstices of 3D aligned carbon nanotube arrays. The aligned CNT structures were prepared by a template assisted non catalytic CVD approach. Herein porous alumina (PAOX) is used as template material in which CNTs are deposited. After removal of PAOX CNT arrays are achieved. We infiltrated PS of two different molecular weights ($21 \cdot 10^3$ and $88 \cdot 10^3$ g/mol) into CNT arrays with 40 and 100 nm tube diameter. For the investigation of the composites we used different experimental techniques like microscopy (TEM, AFM) and scattering (SAXS, SANS). We determined structure of nanotubes (diameter, wall thickness, interactions between tubes) in each step of sample preparation. We are able to see the variation of the scattering during the process of growing CNT in PAOX, removing of the alumina matrix and finally the filling of the system with polystyrene. All these changes were described within a model of cylindrical core-shell particles with two dimensional hexagonal order. Investigation of polymer location in composites shows that filling depends on tube size and molecular weight. Moreover, we applied small angle neutron scattering (SANS) for studying the polymer conformation in composites.

CPP 43.6 Thu 15:30 ZEU 222

Free volume of interphases in model nanocomposites studied by positron annihilation lifetime spectroscopy — Stephan Harms[1], •Klaus Rätzke[1], Franz Faupel[1], Gerald J. 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 nanocomposites by positron annihilation lifetime spectroscopy (PALS) to explore the influence of the interphase nanoscale character of the hydrophobically functionalized filler particles and the nanoscale particle size on positron parameters [1]. A weakly repulsive system, not forming an interphase, was obtained by mixing of low molecular weight poly(ethylene-alt-propylene) (PEP) and hydrophobically modified silica with varying concentration. DSC experiments showed a constant glass transition temperature T_g and a decrease in heat capacity at T_g with increasing filler concentration. In contrast, PALS measurements showed decreasing T_g and a strong drop of the thermal expansion coefficient above T_g. These seemingly conflicting results are due to nanoscale character of filler particles with sizes in the range of the positronium diffusion length. This requires taking into account out-diffusion of positronium from the particles. In particular, the changes on PALS parameters with increasing filler content cannot be attributed to the formation of an interphase with properties different from the polymer matrix.

[1] S. Harms K. Rätzke, F. Faupel, G. J. Schneider, L. Willner, D. Richter in press Macromolecules 2010

CPP 43.7 Thu 15:45 ZEU 222

Unique Splitting Behavior of the C-C Symmetric Stretching Mode as a Raman Signature of Conformational Order of Intercalated Alkyl Chains in Modified Clay Composites — •Patrice Donfack[1], Elena A. Sagitova1[1,2], Kirill A. Prokhorov[2], Kirill V. Vodopianov[2], Goulnara Yu. Nikolaeva[2], Viktor A. Gerasin[3], Nadezhda D. Merekalova[3], Arnulf Materny[1], Evgeny M. Antipov[3], and Pavel P. Pashinin[2] — [1]Center of Functional Materials and Nanomolecular Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany — [2]A.M. Prokhorov General Physics Institute of RAS, Moscow, Russia — [3]A.V. Topchiev Institute of Petrochemical Synthesis of RAS, Moscow, Russia

A specific conformational insight into clay modified by alkylammonium salts is presented. It is associated with the splitting of the symmetric C-C stretching mode at ≈ 1128 cm^{-1} into two bands at 1128 and 1139 cm^{-1} in the Raman spectra of sodium montmorillonite clay modified by alkylammonium surfactants, such as cetyltrimethyl ammonium bromide. We demonstrate that this splitting appears if two trans-segments of nonequivalent lengths and terminal groups coexist for the chains of the alkylammonium ions embedded into the clay interlayer space. Interestingly, this correlates with the conformational reorganization of alkylammonium molecules confined within clay galleries, as a function of the modifier content. Moreover, we show that the integral intensity ratio, $I_{(CH2)}/I_{(705)}$, allows a rapid and nondestructive quantification of the content of alkylammonium ions in the modified clays.

15 min. break

CPP 43.8 Thu 16:15 ZEU 222

Fabrication, Characterization of Multifunctional Tetrapod-ZnO/Polymer Composites for Bioinspired Applications — •Xin Jin, Xinwei Zhu, Sebastian Wille, Arnim Schuchardt, Yogendra Kumar Mishra, and Rainer Adelung — Functional Nanomaterials, Institute of Materials Science, CAU Kiel, Germany

Composite materials design is a fascinating research subject because of the challenge to combine the functionalities of each component and simultaneously give improved properties to the entirety. In biomedical researches, polymers composites play a key role as hard tissue restoratives, like prosthetics, dental implants, etc. One of the most important methods to improve the performance of polymers composite, is to alter the type, amount and size of the filler material. In this work, composites of tetrapods-ZnO micro/nano-particles embedded in PDMS matrix are fabricated. Tensile tests, photon-responsive IV characterization and wettability tests are performed. The results show favorable change in mechanical and electrical properties induced by the special shape of filler. The mechanism of reinforcement is discussed. Researches of this composite material in bio-inspired adhesion applications are in progress. Experiments of tetrapod-ZnO as fillers for dental polymer are also performed.

CPP 43.9 Thu 16:30 ZEU 222

Structure formation during evaporation of a droplet of PEG coated gold nanoparticles on a heterogeneous surface of block copolymers- an in situ μGISAXS combined with ellipsometry study — •Mottakin M. Abul Kashem[1], Volker Körstgens[2], Monika Rawolle[2], Adeline Buffet[1], Gerd Herzog[1], Matthias Schwartzkopf[1], Gunthard Benecke[1], Jan Perlich[1], Rainer Gehrke[1], Peter Müller-Buschbaum[2], and Stephan V. Roth[1] — [1]DESY, Hamburg, Germany — [2]TU München, Physik Department, LS Funkt. Mat., Garching, Germany

We have investigated the nanostructures formed on top of a block copolymer film surface during evaporation of the solvent of a dispersion of gold nanoparticles coated with PEG ligands. The copolymer film contained regular array of PMMA domains in the matrix of PS [1].Presence of ligands can, in the one hand, enhance the selectivity of adsorption and in the other hand, can slow down the migrational flow of the nanoparticles. As a result, several phenomena including selective adsorption, evaporation induced multiscale nanostructures formation and mesoscopic crystallization can be observed [2]. All these open questions have been investigated with in situ micro-beam grazing incidence small angle X-ray scattering (in situ μGISAXS) in combination with in-situ ellipsometry [3, 4] at P03 (MiNaXS) beamline of PETRA III storage ring of HASYLAB at DESY, Hamburg, Germany. [1] Abul Kashem et. al. Macromolecules, 42, 6202 (2009). [2] Roth et. al. Langmuir, 26, 1496 (2010). [3] Müller-Buschbaum, P. Anal. Bioanal. Chem. 376, 3 (2003). [4] Körstgens et. al.Anal. Bioanal. Chem. 396, 139 (2010).

CPP 43.10 Thu 16:45 ZEU 222

Gold Nanoparticles Decorated with Oligo(ethylene glycol) Thiols: Protein Resistance from Single Particle to Superlattice — •Fajun Zhang[1], Maximilian W. A. Skoda[2], Robert M. J. Jacobs[3], Claire Pizzey[4], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany — [2]ISIS, Rutherford Appleton Laboratory, Chilton, UK — [3]Department of Chemistry, Chemistry Research Laboratory, University of Oxford, UK — [4]Diamond Light Source, UK

Self-assembled monolayers (SAM) with oligo(ethylene glycol) (OEG) termination are of great importance in biomedical applications due to their protein resistance property. We have successfully prepared OEG-thiol decorated gold colloids and studied various interactions, stability and aggregation kinetics of colloid in the mixture with proteins by SAXS and UV-vis spectroscopy [1]. The results show that the protein resistance of the OEG SAM is maintained at curved interfaces. It is also shown that the colloids lose their stability and form aggregates upon adding protein above a critical concentration due to the depletion-attractive interaction [1]. The stability of the mixtures of the functionalized AuNP and proteins in solution strongly depends on the nature of added salts, which follow the Hofmeister series [1]. Further, a superlattice of SAM coated AuNP on a substrate is obtained, which provides a new model interface with protein resistance property. SAXS measurements indicate an FCC structure of the superlattice.

[1] F. Zhang, et al. J. Phys. Chem. A 2007, 111, 12229. Eur. Biophys. J. 2008, 37, 551. J. Phys. Chem. C 2009, 113, 4839.

CPP 43.11 Thu 17:00 ZEU 222

Structure and dynamics of poly ethylene glycol grafted gold nanoparticles studied by neutron scattering — •Marco Maccarini — Institut Laue Langevin, Grenoble, France

Polymer-capped gold nanoparticles (AuNP) have many peculiar aspects like quantum size effects and single electron transitions. Their properties are highly dependent on their size and shape and upon spatial relationship of one particle to another. Coating nanoparticles with polymers tethered to their surface by means of specific ligands stabilizes them, and allows functionalization for specific applications in nanotechnologies, biology and biomedical studies. We studied the structure and the dynamics of a key class of polymer-capped AuNP, those coated with poly ethyleneglycol (PEG). A novel synthesis was developed by ligand exchange procedure, which ensure the production of NP with little excess of functionalizing ligand and high stability. The structure PEG AuNP were studied by combining small angle neutron scattering as a function of temperature, and of the length of the interfacial polymer chains. PEG Au NP functionalized with short (PEG400) and long (PEG2000) polymer reflected substantial differences in the structure of the polymer at the interface. The dynamics of PEG AuNP in the nanosecond timescale was also studied by neutron spin echo (NSE) spectroscopy. NSE experiments showed two dynamical processes, one related to the translational diffusion of the nanoparticles, and a faster due to internal motion of the polymer chains. For comparison, NSE experiments were performed on PEG2000 polymer in solutions. Analogies and differences between free and anchored polymer will be discussed.

CPP 43.12 Thu 17:15 ZEU 222

Surface Layering of suspended Au-Nanoparticles — •Volker Schön[1], Patrick Huber[1], Philip Born[2], and Tobias Krauss[2] — [1]Saarland University, 66123 Saarbrücken, Germany — [2]Leibniz-Institut für Neue Materialien gGmbH, 66123 Saarbrücken, Germany

We present x-ray reflectivity measurements performed on our home made spectrometer showing that thiolated Au-nanoparticles suspended in toluene constitute layers at the toluene-air interface.

The experiments were performed in a closed cell with virtually no evaporation taking place, the height of the liquid being stable over several days.

The number and density of these layers strongly depends on the concentration of said suspensions and is also influenced by temperature.

CPP 43.13 Thu 17:30 ZEU 222

In situ GISAXS investigation of Gold-sputter deposition onto colloidal polymer templates prepared by airbrush coating — •Adeline Buffet[1], Gerd Herzog[1], Matthias Schwartzkopf[1], Jan Perlich[1], Mottakin Abul Kashem[1], Volker Koerstgens[2], Peter Mueller-Buschbaum[2], and Stephan V. Roth[1] — [1]DESY, Notkestr. 85, 22607 Hamburg, Germany — [2]TU Muenchen, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany

New applications for metal-polymer nanocomposites have emerged in the field of organic optics and electronics [1], or in the field of hybrid sensors [2]. Therefore, much effort has been put to better understand the growth process and structural transition of nanocomposites [3]. We investigated in situ the growth of a sputter-deposited ultra-thin gold film on top of a pre-structured colloidal polymer template using grazing incidence small-angle X-ray scattering (GISAXS). The underlying colloidal polymer template was deposited by using the novel technique of airbrush-spray coating, allowing for the installation of stripe-type trapezoidal pattern consisting of 3D hexagonally closed-packed colloids [4]. We present our findings on the formation of gold nanoclusters on top of the individual polymer colloids and give an outlook how to open a promising route to generate plasmon waveguides and photonic crystals, e.g. anti-reflective coatings. [1] Biswas, B. et al. Vacuum Technology & Coating 1, 54 (2006). [2] Wolkenhauer, M. et al. Appl. Phys Lett. 79, 054101 (2006). [3] Metwalli, E. et al. Langmuir 24, 4265 (2008). [4] Buffet, A. et al. Adv. Eng. Mat. Journal, Accepted (2010)

CPP 43.14 Thu 17:45 ZEU 222

Highly uniform SERS substrates formed by wrinkle-confined drying of gold colloids — Nicolás Pazos-Pérez[1], Alexandra Schweikart[1], Andrea Fortini[1], Matthias Schmidt[1], Ramon Álvarez-Puebla[2], Luis M. Liz-Marzan[2], and •Andreas Fery[1] — [1]PC II and TP II, University of Bayreuth, Germany — [2]PC, University of Vigo, Spain

Metallic nanoparticles, exhibit electric and optical properties which are size and shape dependent. Therefore, they are ideal candidates for many applications. Big effort has been put in developing new methods to control their shape and size. These achievements allow us to fine tune the materials properties in order to use them for a desired application. However, the lack of capability to form organized structures is still a very important challenge in order to use these materials in many applications. In this work we report a novel method to structure, in a macroscale range, arrays of organized gold colloids into 1 and 2D linear parallel arrays which are highly uniform substrates for Surface Enhanced Raman Scattering (SERS). These structures were fabricated through self-assembly of gold nanoparticles upon solution-drying in a periodic confining structure. The technique leads to uniform, parallel linear nanoparticle arrays with the precise arrangement defined through the dimensions of the particles and the grooves. Moreover, the good reproducibility of these structures among big areas, make them perfect candidates as ultrasensitive substrates for SERS due to the formation of controlled Hot Spots arrays. Which provide high and uniform SERS enhancement over extended areas.

Topical Talk CPP 43.15 Thu 18:00 ZEU 222

Are nanomaterials safe? Physico-chemical characterization for regulation and for life-cycle assessment of nanocomposites — •Wendel Wohlleben — BASF SE, Polymer Physics Research, 67056 Ludwigshafen

Nanocomposites are the dominating class of nanomaterials to come into consumer contact. For the first time, our comprehensive study addresses a systematic series of thermoplastic and cementitious nanocomposite materials with SiO2, CNT, crystal seeds as embedded nanofillers. We confirm earlier reports that 'chalking', i.e. release of pigments from weathered paints, does occur also for nanocomposites. In contrast, mechanical forces by normal consumer use or do-it-yourself sanding do not disrupte nanofillers from their matrix. Combining SEM, AUC, XPS, SIMS, diffraction we find no free nanofillers up to the detection threshold of 100 ppm. Sanding powder particles still contain the nanofillers. And yet, is there a hazard from these aerosols? We perform in vivo studies in rats and quantify physiological effects of degradation products. A summarizing risk assessment confirms that nanocomposites are indeed safe in consumer settings.

However, occupational safety against inadvertant inhalation of dust must be established by suitable methods for containment of specific nanomaterials. Physico-chemical characterization is key to identify such nanomaterials and to understand their biophysical interactions in a physiological environment.

CPP 44: Micro- and Nanofluidics I

Time: Thursday 14:00–18:00 Location: ZEU 160

CPP 44.1 Thu 14:00 ZEU 160

Enantioselective separation by an asymmetric flow profile — •Florian J. Lorenz[1], Lukas Bogunovic[1], Ralf Eichhorn[2], Dario Anselmetti[1], and Jan Regtmeier[1] — [1]Bielefeld University, Bielefeld, Germany — [2]NORDITA, Stockholm, Sweden

The pharmaceutical use of homochiral chemicals is of great interest, because they have different physiological responses in organisms, because of the chiral selectivity in biological systems.

Since abiotic synthesis strategies often render an enantiomeric mixture (so called racemate), the racemate-splitting into pure enantiomers is one of the main challenges. To date, however, this is often realized by chromatography- and electrophoresis-separation-methods, with the great disadvantage that specifically designed chemical selectors are needed.

We present an alternative physical method, selector-free and continuously working, to separate enantiomers at the micrometer scale. It is based on an asymmetric flow profile within a microfluidic Lab-On-a-Chip (LOC) platform with broken spatial symmetry. We could demonstrate that the enantiomers are separated within the micro-channel and can be harvested in different reservoirs at the end.

Currently we explore the possibility to further miniaturize those devices for nanoscale separation of chiral molecules.

CPP 44.2 Thu 14:15 ZEU 160

AC driven nanopump — •Klaus F. Rinne, Stephan Gekle, Douwe Jan Bonthuis, and Roland Netz — Physik Department, TU München, Germany

We present a novel mechanism for pumping water through a (20,0) carbon nanotube (CNT) without requiring external pressure gradients. Using molecular dynamics simulations (with the LAMMPS package) we show that pumping can be achieved through a periodic electric field. The electrical energy of the water dipoles is translated into particle motion via translation-orientation-coupling. We determine the pumping efficiency consistent with thermodynamics. Our system is simple enough that it could be experimentally realizable and might serve as a basis for microscale filtration systems.

CPP 44.3 Thu 14:30 ZEU 160

A microfluidic ratchet device for the controlled and tuneable separation of microparticles — •Lukas Bogunovic[1], Ralf Eichhorn[2], Jan Regtmeier[1], Dario Anselmetti[1], and Peter Reimann[1] — [1]Bielefeld University, Bielefeld, Germany — [2]NORDITA, Stockholm, Sweden

Standard biotechnological separation techniques - such as gel electrophoresis - are often restricted to a separation criterion that is unchangeably implemented during fabrication. Therefore a new microfluidic device, based on a dielectrophoretic (DEP) ratchet design, has been designed and characterized [1]. It allows the dynamic and selective adaption of the separation criterion and direction of migration during operation. As a proof-of-concept, we demonstrate the separation of one arbitrary micro bead species out of three different kinds with freely selectable direction of migration for each species. The device consists of a straight microfluidic channel structured with an array of triangles. Here, DEP traps are created by an alternating voltage U_{AC} while a constant voltage U_{DC} drives negatively charged parti-

cles with diameters d_1=1.1μm, d_2=1.9μm and d_3=2.9μm through the channel by electrophoresis (EP). Depending on the relative strengths of EP and DEP forces, a selection of particle types that will be trapped and those, which will still be transported can be archived. Combining these system states to a tailored driving protocol leads to the desired separation task.
[1] L. Bogunovic et al. "A tuneable microfluidic ratchet for particle sorting", submitted 2010

CPP 44.4 Thu 14:45 ZEU 160

Directed transport of DNA polymer molecules in micro- and nanochannels — •Ronny Sczech[1], Steffen Howitz[2], and Michael Mertig[1] — [1]Technische Universität Dresden, 01062 Dresden, Germany — [2]GeSiM, Bautzner Landstrasse 45, 01454 Großerkmannsdorf, Germany

DNA molecules can be transported in a nanochannel with help of both electrophoretic and hydrodynamic flow. Transport experiments and theoretical considerations suggest an interaction of electrophoresis, electro-osmosis, and the unique statistical properties of confined polymers. Besides that, the confinement of the device is crucial since it influences the electric field in the nanochannel.

Nanofluidic channels in polydimethylsiloxane (PDMS) were formed by classical nanoimprinting technology combining micro- and nanofluidic features. The feasibility of those hybrid micro- and nanofluidic structures for single molecule observation and manipulation was demonstrated by introducing single molecules of λ-DNA into the channels using optimized parameters for the applied potential and flow.

It was possible to show the manipulation of λ-DNA molecules in PDMS nanochannels with a cross section ≤ 1 μm using epifluorescence microscopy. Once stabilized inside a nanochannel the free diffusion of individual λ-DNA molecules were observed. Diffusivity was compared with previous studies that concentrated on nanoslits and checked for adaptability to blob theory and reflecting rod theory. In this context, electrokinetic concentration of the λ-DNA were observed during the application of an sufficient electrical field.

CPP 44.5 Thu 15:00 ZEU 160

Omniphobicity Scrutinized with a Phase-Field Approach — •Walter Mickel[1,2] and Thierry Biben[1] — [1]Université de Lyon, F-69000, Lyon, France; Université Lyon 1, F-69622, Villeurbanne, France; CNRS, UMR5586, Laboratoire PMCN — [2]Institut für Theoretische Physik, Friedrich-Alexander Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen, Germany

Spreading liquids on a rough surface with pillars may result in a penetrated Wenzel-state where liquid enters the grooves or a fakir state with air-pockets suspending the liquid above. On micronic scales this behavior is very well described with the Wenzel- and Cassie-Baxter laws. According to this theory hydrophobic materials are needed to obtain superhydrophobic states due to the roughness induced amplification of the hydrophobicity. An inversion of the wetting behavior due to roughness, could not be explained by the theory. However experiments from Ramos[1] and simulations from Daub[2] showed that intrinsic hydrophilic materials could render hydrophobic with appropriate surface structures. Such materials are called omniphobic.

We study the mechansims which lead to omniphobic substrates with a phase-field model[3] coming from mesoscale to nanoscale wetting. With this model we investigate the free energy landscape to quantify metastabilities and dynamic transitions. Further we report the impact of several roughness parameters on the wetting inversion. We discuss the capillary filling of grooves and show a mesoscopic wetting theory.

[1] S. Ramos, Langmuir 26 (2010) 5141-6 [2] C.D. Daub, Faraday Discussions 146 (2010) 67-77 [3] T. Biben, PRL 100 (2008) 186103

CPP 44.6 Thu 15:15 ZEU 160

Electrical switching of wetting states on superhydrophobic surfaces: a route towards reversible Cassie-to-Wenzel transitions — Gor Manukyan, Oh Jung Min, van den Ende Dirk, Lammertink Rob, and •Mugele Frieder — University of Twente, MESA institute, Enschede, The Netherlands

We demonstrate that the equilibrium shape of the composite interface between superhydrophobic surfaces and drops in the Cassie state under electrowetting is determined by the balance of the Maxwell stress and the Laplace pressure. Energy barriers due to pinning of contact lines at the pillar edges control the transition from Cassie to the Wenzel state. Barriers due to the narrow gap between adjacent pillars control the lateral propagation of the Wenzel state. Suitable engineering of surface and electrode geometries allows for reversible local switching between the two wetting states.

CPP 44.7 Thu 15:30 ZEU 160

MD simulation of polymer droplets on super-hydrophobic substrates — •Nikita Tretyakov and Marcus Müller — Georg-August Universität, Göttingen

We study coarse-grained polymer liquids on super-hydrophobic substrates by Molecular Dynamics simulation. The systems under investigation consist of a polymer droplet on a spatially structured corrugated substrate. The temperature is controlled by DPD thermostat which locally conserves the momentum. The values of the contact angle are dictated by the substrate-liquid interaction and the geometry of the substrate corrugation. Cassie and Wenzel states are observed by changing the amplitude of Lennard-Jones interaction between polymer chains and substrate's atoms.

Applying the body force onto droplet's molecules we study dynamical properties of the system. Spatial corrugation of the substrate initiate the pinning of the droplet's contact line. The energy barriers needed to be overcome for depinning are estimated. The fluctuations of the contact line providing information on capillary waves on the droplet's surface are explored. The energy dissipations due to the presence of the substrate are calculated. Directed motion caused by asymmetry of the substrate corrugation is studied.

CPP 44.8 Thu 15:45 ZEU 160

Anisotropic wetting behavior on groove patterns — •Ciro Semprebon[1], Carsten Herrmann[2], Ralf Seemann[2], Stephan Herminghauss[1], and Martin Brinkmann[1] — [1]MPI for Dynamics and Self-Organization, Goettingen — [2]Universitat des Saarlandes, Saarbrucken

We investigate theoretically and experimentally the shape of small liquid droplets condensing on a substrate decorated with periodic micropatterns of parallel grooves. Depending on the pattern geometry and substrate wettability these droplets may either grow solely in the direction of the grooves forming elongated filaments, or spread anisotropically in both directions. In the spreading regime the droplet eccentricity oscillates as the number of wet grooves increases, ultimately reaching a scale invariant shape with a well defined anisotropy. The boundaries of the stability of filaments can be computed from an analytical model and depend on the number of grooves which are wet. Generally we find that the region of stability of filaments is smaller for filaments wetting a larger number of grooves. For the particular case of V-grooves the filaments may undergo either a Rayleigh-Plateau instability or lateral depinning of the contact line. The scale invariant shape can be described with a numerical model for liquid droplets confined to a single wettable stripe.

15 min. break

CPP 44.9 Thu 16:15 ZEU 160

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

Transport and flow phenomena in porous media occur 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. We discuss the relationship between permeability and porosity near and far off the percolation threshold of different random structures.

CPP 44.10 Thu 16:30 ZEU 160

Dynamics of Forced-Imbibition in Porous Media — •Kamaljit Singh[1,2], Hagen Scholl[2], Marco Di Michiel[3], Mario Scheel[3], Stephan Herminghaus[1], and Ralf Seemann[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, D-37073 Goettingen, Germany — [2]Saarland University, D-66041 Saarbruecken, Germany — [3]European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble, France

We used ultrafast X-ray micro-tomography at the European Synchrotron Radiation Facility (ESRF, ID15) to observe the three-dimensional dynamic behaviour of water-oil fronts during a water flood into an initially oil filled porous medium. This type of multiphase flow is similar to a situation which can be found for oil recovery or soil decontamination. We characterised the pore and throat parameters of the porous media, and analysed the water-oil front behaviour at pore scale for various factors, including wettability of porous matrix, flow velocity and porosity. The dynamic experiments reveal that in an oil-wet medium, the water-oil front is more compact, however the front in a water-wet porous medium progresses in elongated fingers. The fingering in water-wet porous medium results in a higher final residual oil saturation after a complete water flood due to by-passing of several oil-filled pore pockets. We will compare the experimental results for various parameters with models developed from pore-throat characteristics.

CPP 44.11 Thu 16:45 ZEU 160

Phase behaviour and rheology of the liquid crystal 8OCB in confinement — •Dominik Gerstner, Simon Gruener, and Patrick Huber — Experimental Physics, Saarland University, Saarbrücken, Germany

To examine the hydrodynamic properties of the liquid crystal 8OCB in nanoscale confinement, we measured the time dependence of its capillary rise into porous Vycor glass. Porous Vycor is a monolithic silica glass, permeated by a random network of pores with a mean diameter of approximately 7 nm. The capillary rise was monitored by the mass uptake $m(t)$ of the system. We observed the typical Lucas-Washburn behaviour for all our measurements, which suggests the validity of bulk hydrodynamics even in such strong confinement. However, the shear viscosity minumum, appearing at the bulk isotropic-nematic transition of 8OCB, is found to be absent. We explain this with the formation of a paranematic phase, i.e. the continuous evolution of molecule alignment due to the ordering effects of the narrow pores. The evolution of the paranematic order can also be seen in ^{13}C neutron magnetic resonance spectroscopy and differential scanning calorimetry measurements on 8OCB in a porous Vycor host.

CPP 44.12 Thu 17:00 ZEU 160

Wetting of liquid-crystals on flat surfaces. The role of substrate anchoring. — •Manuel Greschek[1] and Martin Schoen[1,2] — [1]Stranski-Laboratorium für Physikalische und Theoretische Chemie, Fakultät für Mathematik und Naturwissenschaften, Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, GERMANY — [2]Department of Chemical and Biomolecular Engineering, Engineering Building I, Box 7905, North Carolina State University, 911 Partners Way, Raleigh, NC 27695, USA

Predicting the behaviour of liquid crystals in confinement plays an important role in developing novel nanotechnological devices such as biosensors. Using grand canonical Monte Carlo simulations we investigate the impact of different anchoring scenarios on the wetting behaviour of a model liquid-crystal confined by a mesoscopic slit-pore. The intermolecular fluid-fluid interaction is modeled by a modified Lennard-Jones potential with an orientation-dependent attractive term. Different anchoring scenarios are described by an anchoring function $g(\hat{\mathbf{u}})$, that discriminates energetically between different orientations of a molecule with respect to the substrate plane. Depending on the specific anchoring scenarios the fluid may or may not wet the solid substrate where wetting may involve an orientation dependent prewetting transition. The thickness of the wetting layer is shown to depend on the anchoring function as well.

CPP 44.13 Thu 17:15 ZEU 160

Mechanical Properties of Wet Granulates — •Somnath Karmakar[1], Marc Schaber[1], Mario Scheel[2], Marco Di Michiel[2], Stephan Herminghaus[3], 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 small amounts of a wetting liquid to dry granular matter typically leads to a substantial increase of the mechanical stiffness of the granular media. This arises due to the formation of capillary bridges, exerting an attractive force between individual grains. We study the mechanical properties, i.e. yield stress, tensile strength and critical fluidization acceleration of wet granular materials with different wettability using glass and basalt beads and sand grains at various liquid contents. The mechanical properties are probed for various experimental conditions and surprisingly the wetting liquid might act as a lubricant for a granulate sheared at large absolute pressure. Moreover, we experimentally find for a wetting system a yield stress that is depending on the applied shear frequency. For a granular system with low wettability however, the yield stress is independent of the shear frequency. By time resolved X-ray tomography experiments we can explain this behavior by a liquid exchange process occurring between the individual liquid morphologies emerging in wettable granulates but which is not observed in granulates with low wettability.

CPP 44.14 Thu 17:30 ZEU 160

Dielectric response of interfacial water — •Stephan Gekle, Douwe Jan Bonthuis, and Roland Netz — Physik Department, TU München, Germany

Water at interfaces or in confinement often exhibits unique properties. In this talk we focus on the dielectric response to an external frequency-dependent electric field and outline possible consequences for dielectric heating and electro-osmotic flow. Using molecular dynamics computer simulations, we further show how the interfacial behavior is related to a nonlocal dielectric function which can be observed even in bulk water.

CPP 44.15 Thu 17:45 ZEU 160

Drop Impact on Free-Standing Surfactant Films — •Daniela Fell[1,2], Mordechai Sokuler[1,2], Andreas N. Lembach[2,3], Chuanjun Liu[1,2], Elmar Bonaccurso[2], Günter K. Auernhammer[1], and Hans-Jürgen Butt[1,2] — [1]Max Planck Institute for Polymer Research, 55128 Mainz — [2]Center of Smart Interfaces, 64287 Darmstadt — [3]Institute of Fluid Mechanics and Aerodynamics, 64287 Darmstadt

We investigate the influence of drop composition on the drop's behavior during impact. The drops of either water or aqueous surfactant solution had a diameter of (2.4 ± 0.4) mm and impacted with a velocity up to 1.3 m/s. As surfactants the anionic sodium dodecyl sulfate (SDS) and the cationic cetyl trimethyl ammonium bromide (CTAB) were used. Pure water drops impacting on surfactant films showed coalescence, bouncing, passing, partial bouncing, and partial passing. When surfactant was added to the drop, partial passing was suppressed and coalescence was replaced by (partial) bouncing.

We interpret the different phenomena based on the repulsive hydrodynamic force arising when the air has to flow out of the closing gap between the two liquid surfaces. This repulsion is influenced by the hydrodynamic boundary condition at the air-water interface. For a mobile interface represented by water drops impacting on surfactant films the outflow of air should be faster than for a no-slip boundary condition represented by both liquids containing surfactant. The boundary condition change from mobile to no-slip condition leads to stronger hydrodynamic repulsion in case of impacting surfactant drops.

CPP 45: Colloids and Complex Liquids III - External Fields

Time: Thursday 17:15–18:00 Location: ZEU 114

CPP 45.1 Thu 17:15 ZEU 114

Structure formation and dynamics of dipolar colloids in rotating fields — •Sebastian Jäger and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We investigate suspensions of colloidal dipolar particles that are exposed to external rotating fields. Given suitable system parameters these systems form layered structures. We are mainly interested in the dynamics of the colloidal particles and the question for which field strengths and frequencies layer formation occurs. To explore these matters, we employ computer simulations, most notably Brownian (Langevin) dynamics simulations, which we supplement by semi-analytical considerations. In particular, we propose a simple theory that describes layer formation in a density functional framework [1].

[1] S. Jäger and S. H. L. Klapp, in preparation.

CPP 45.2 Thu 17:30 ZEU 114

Meniscus of a ferrofluid around a vertical cylindrical wire carrying electric current — •Kathrin May, Thomas John, and Ralf Stannarius — Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg

We investigate quantitatively a common presentation experiment in ferrofluids - the shape of a meniscus in the field of a current-carrying wire. Neglecting the surface tension, the height of the free surface profile of the ferrofluid can be determined to $h \propto r^{-2}$, where r is the distance to the center of the wire [1]. The influence of the surface tension has been discussed theoretically in [2]. Here we compare these results with experimental data. All material parameters are known, therefore no fitting parameters are used in comparisons. The significant differences between the model in [1] and experimental results can be explained by the influence of the surface tension.

[1] R. E. Rosensweig, Ferrohydrodynamics, Dover Publications, New York, 1997.

[2] Th. John et al., J. Magn. Magn. Mater. 309, 31 (2007).

CPP 45.3 Thu 17:45 ZEU 114

Ground states of ferrofluid monolayers in the presence of an external magnetic field — •Taisia Prokopieva[1,2], Victor Danilov[1], Sofia Kantorovich[1,2], and Christian Holm[2] — [1]Ural State University, Lenin av. 51, Ekaterinburg, 620000, Russia — [2]Institute fuer Computerphysik, Universitaet Stuttgart, Pfaffenwaldring 27, 70569, Stuttgart, Deutschland

We study the system of magnetic dipolar particles the centres of which are confined in one plane. Particles themselves are free to rotate, thus forming a so called quasi-2D monolayer system [Klokkenburg et al, Phys. Rev. Lett., 2006]. Computer simulations and theoretical studies of these systems were actively performed in the last years both at room temperatures [Kantorovich et al, PCCP, 2008] and at the ground state [Prokopieva et al, Phys. Rev. E, 2009]. All these works however did not consider the possibility to control the structural transitions in such a system by the direction and intensity of the external magnetic field. The latter opens a wide range of new effects. Here we present the combination of Monte Carlo simulated annealing and theoretical modeling to describe the response of a ferrofluid monolayer to the applied magnetic field at low temperature. Our investigations show the dominant role of the magnetic correlations within the monolayer plane, which we characterise in terms of initial magnetic susceptibilities.

CPP 46: Micro- and Nanofluidics II

Time: Friday 10:30–13:00 Location: ZEU 222

Topical Talk CPP 46.1 Fri 10:30 ZEU 222

Droplet-based microfluidics and the dynamics of emulsions — •Jean-Christophe Baret — Max-Planck Institute for Dynamics and Self-organization

Emulsions are complex fluids already involved for a long time in a wide-range of industrial processes, such as, for example, food, cosmetics or materials synthesis [1]. More recently, applications of emulsions have been extended to new fields like biotechnology or biochemistry where the compartmentalization of compounds in emulsion droplets is used to parallelize (bio-)chemical reactions [2,3]. Interestingly, these applications pinpoint to fundamental questions dealing with surfactant dynamics, dynamic surface tension, hydrodynamic interactions and electro-hydrodynamics. Droplet-based microfluidics is a very powerful tool to quantitatively study the dynamics of emulsions at the single droplet level or even at the single interface level: well-controlled emulsions are produced and manipulated using hydrodynamics, electrical forces, optical actuation and combination of these effects. We will describe here how droplet-based microfluidics is used to extract quantitative informations on the physical-chemistry of emulsions for a better understanding and control of the dynamics of these systems.

[1] J. Bibette et al. Rep. Prog. Phys., 62(6), 969-1033 (1999) [2] A.D. Griffiths and D. Tawfik, Trends in Biotechnology, 24(9), 395-402 (2006) [3] J.-C. Baret et al. Chem. Biol., 17(5), 528-536 (2010)

CPP 46.2 Fri 11:00 ZEU 222

Structural Transitions in a Two-Dimensional Microfluidic Crystal — •Jean-Baptiste Fleury[1], Ohle Caussen[2], Stephan Herminghaus[2], Martin Brinkmann[2], and Ralf Seemann[1,2] — [1]Saarland University, Saarbrücken, Germany — [2]Max Planck Institute for dynamic and Self-Organization, Goettingen, Germany

To understand the fundamental principles of droplet packing and manipulation in microfluidic channels we explore the static arrangement of a train of monodisperse water-in-oil emulsion droplets trapped in a straight, quasi two dimensional microfluidic channel with flat rectangular cross section. The length of the droplet train at constant droplet number can be varied by liquid plugs which act as two movable pistons. In this experimental setting we control the static compressive force applied by these plugs and allow the emulsion to mechanically equilibrate by an exchange of the continuous phase with a reservoir. As a result of the changing longitudinal confinement the droplets self-organize in different packing geometries, depending on their size, which can be distinguished by the topology of their contact network. These experimental results are in good quantitative agreement with our analytical calculations of the droplet arrangement, based on minimization of the interfacial energy. The theoretical predictions of droplet organization in different packing geometries also holds true when the structure is flowing in microfluidic channels. Indeed, these flowing structures self organize in periodic lattices that correspond to local minima of the relevant energy functional already discuss in the static case.

CPP 46.3 Fri 11:15 ZEU 222

Deformation of particle-stabilized droplets in multicomponent fluids — •Stefan Frijters and Jens Harting — Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands

Traditionally, enhanced oil recovery processes often employ surfactants to improve oil yield. In this project, nanoparticles are considered as an alternative to these surfactants. To determine in which ways these particles might be useful we need to understand how they modify the properties of a droplet of fluid suspended in another fluid. We present a simulation algorithm based on a multicomponent lattice Boltzmann model to describe the solvents combined with a molecular dynamics solver for the description of the solved particles. We have the ability to tune numerous relevant parameters of the system, such as particle sizes and wettability and surface tensions between the fluids and we use this ability to study the behaviour of fluid droplets stabilized by particles when subjected to shear. We then consider how these effects compare to those of surfactants.

CPP 46.4 Fri 11:30 ZEU 222

Influence of the solid/liquid interface on the flow dynamics of unentangled polymer melts — •Mischa Klos, Matthias Lessel, Oliver Bäumchen, and Karin Jacobs — Saarland University, Department of Experimental Physics, D-66041 Saarbrücken

Due to downsizing of microfluidic devices, the solid/liquid interface becomes more and more influential for liquid flow. In classic hydrodynamics, the velocity profile of a liquid flowing through a tube or over a surface extrapolates to zero close to a wall. By applying a hydrophobic coating to the solid surface it is possible to create a finite velocity of the liquid at the solid/liquid interface, known as slippage. Slippage is characterized by the extrapolation length of the flow profile, called slip length. In our experiments, liquid flow is induced by an internal driving force which drives the dewetting of thin polymer films on hydrophobic substrates. The slip length can be extracted by monitoring the dewetting dynamics of the emerging holes in the film or by characterizing the shape of the surrounding rim. Aside from the strong impact of inter-chain entanglements on slippage, also the type of hydrophobic substrate influences the slip length. We show results for thin polystyrene films flowing over an amorphous polymeric coating (AF1600) and different types of self-assembled monolayers of silanes. The AF1600 induces nearly no slip at the solid/liquid interface, in contrast to the silan surfaces, where the slip length reaches values from several hundreds of nanometers up to micrometers. We investigate whether slippage varies with the silane's chain length, its structure on the molecular level and the surface energy.

CPP 46.5 Fri 11:45 ZEU 222

Simulations of slip flow on rough and nanobubble-laden surfaces — •Jens Harting[1,2], Christian Kunert[2], and Jari Hyväluoma[3] — [1]Department of Applied Physics, Eindhoven University of Technology, Den Dolech 2, NL-5600MB Eindhoven, The Netherlands — [2]Institute for Computational Physics, University of Stuttgart, Pfaffenwaldring 27, D-70569 Stuttgart, Germany — [3]MTT Agrifood Research Finland, FI-31600 Jokioinen, Finland

On microstructured hydrophobic surfaces, geometrical patterns may lead to the appearance of a superhydrophobic state, where gas bubbles at the surface can have a strong impact on the fluid flow along such surfaces. In particular, they can strongly influence a detected slip at the surface. We present two-phase lattice Boltzmann simulations of a flow over structured surfaces with attached gas bubbles and demonstrate how the detected slip depends on the pattern geometry, the bulk pressure, or the shear rate. Further, we present recent results from the modeling of AFM based experiments for slip measurements and the investigation of fluid-surface interactions.

CPP 46.6 Fri 12:00 ZEU 222

Quantitative Analysis of Fluorescence Cross Correlation Spectroscopy Data for the Study of Hydrodynamics near Surfaces — Roman Schmitz[1], Stoyan Yordanov[1], Hans-Juergen Butt[1], Kaloian Koynov[1], and •Burkhard Duenweg[1,2] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Dept. of Chemical Engineering, Monash University, Melbourne, Australia

We present a new method of data analysis for the interpretation of fluorescence cross correlation spectroscopy measurements in total internal reflection, from particles immersed in hydrodynamic flows near surfaces. Brownian Dynamics simulations are used to produce auto- and cross-correlation curves with defined input values of parameters like shear rate, slip length, particle diffusion constant, etc. These curves are directly compared with the corresponding experimental results. The optimum set of parameters, together with the corresponding set of their statistical errors, is the solution of a nonlinear fit problem, which is solved by an importance-sampling Monte Carlo procedure in parameter space. Substantial statistical effort in both the experiments and the numerics produces good agreement between experiment and theory, but also reveals subtle deficiencies in the underlying simulation model. Nevertheless, even the present simple model is already able to produce a fairly reliable bound on the slip length.

CPP 46.7 Fri 12:15 ZEU 222

Mesoscopic simulations of electroosmotic flow and electrophoresis in nanochannels — •Jens Smiatek[1] and Friederike Schmid[2] — [1]Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität, D-55099 Mainz, Germany

We review recent dissipative particle dynamics (DPD) simulations of electrolyte flow in nanochannels. A method is presented by which the slip length δ at the channel boundaries can be tuned systematically from negative to infinity by introducing suitably adjusted wall-fluid friction forces. Using this method, we study electroosmotic flow (EOF) in nanochannels for varying surface slip conditions and fluids of different ionic strength. Analytic expressions for the flow profiles are derived from the Stokes equation, which are in good agreement with the numerical results. Finally, we investigate the influence of EOF on the effective mobility of polyelectrolytes in nanochannels. The relevant quantity characterizing the effect of slippage is found to be the dimensionless quantity $\kappa\delta$, where $1/\kappa$ is an effective electrostatic screening length at the channel boundaries.

CPP 46.8 Fri 12:30 ZEU 222

On the dissipation and oscillatory solvation forces in confined liquids — •Sissi de Beer[1], Wouter den Otter[2], Dirk van den Ende[1], Wim Briels[2], and Frieder Mugele[1] — [1]Physics of Complex Fluids, Twente University, Enschede, the Netherlands — [2]Computational BioPhysics, Twente University, Enschede, the Netherlands

Usually, a fluid is considered as a continuum medium characterized by a well-known density and viscosity. Upon miniaturization of (nano-) fluidic systems down to a height of only a few nanometer, however, the discrete molecular structure becomes visible and the liquid behaves completely different from the bulk. We study the dissipation in confined liquids and show via Atomic Force Microscope measurements and Molecular Dynamics simulations that the dissipation depends highly on the structure of the liquid molecules. When a discrete amount of molecular layers fit between the two confining surfaces the molecules are maximally organized and we find a minimum in the dissipation, while in between the dissipation significantly increases.

CPP 46.9 Fri 12:45 ZEU 222

Energetics of diffusiophoretic motion — •Benedikt Sabass and Udo Seifert — II Institut für Theoretische Physik, Universität Stuttgart, Germany

Small particles, in a viscous medium, propelled through an asymmetric distribution of solutes around them, can be employed for active transport or even as micromotors. For neutral solutes, this motion is termed diffusiophoresis. The asymmetry of solute concentration can be either produced by a chemical reaction on the particle surface (self-propelled swimmer) or it can be externally imposed. Here we discuss energetic aspects of diffusiophoresis [1]. We calculate the efficiency of a self-propelled swimmer in a true steady state for different reaction kinetics. The role of the hydrodynamic efficiency as upper bound to the overall efficiency is stressed. Further, we investigate the energy balance of quasi-stationary descriptions of diffusiophoresis in an externally imposed solute gradient, where the solute convection must be taken into account.

[1] B. Sabass and U. Seifert, Phys. Rev. Lett. 105, 218103 (2010)

CPP 47: Heterogeneous Nucleation and Microstructure Formation (related to SYMF, jointly with MM)

Time: Friday 10:30–12:45 Location: ZEU 160

CPP 47.1 Fri 10:30 ZEU 160

Nanoparticle solution casting kinetics on colloidal templates - an in-situ microbeam GISAXS and ellipsometry study — •Stephan V. Roth[1], Adeline Buffet[1], Mottakin Abul Kashem[1], Gunthard Benecke[1,2], Rainer Gehrke[1], Gerd Herzog[1], Volker Koerstgens[3], Jan Perlich[1], Monika Rawolle[3], Andre Rothkirch[1], Matthias Schwartzkopf[1], and Peter Mueller-Buschbaum[3] — [1]Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, D-22607 Hamburg, Germany — [2]MPIKG Golm, Abt. Biomat., Wissenschaftspark Potsdam-Golm, D-14424 Potsdam, Germany — [3]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany

Nanoparticle solution casting is a very efficient process to produce large scale nanostructured layers [1] which are applied in optical or sensor technology [2]. We investigated the self-assembly process of gold nanoparticles during solution casting on a colloidal polymeric template. The template was installed by spin-coating and further nanostructured by toluene treatment prior to solution casting. In order to follow the different stages of self-assembly during evaporation of the solvent, we combined imaging ellipsometry [3] and microbeam grazing incidence small-angle x-ray scattering (μGISAXS) at the beamline MiNaXS (P03) of DESY, Hamburg. Thereby we are able to image the structure formation of the gold nanoparticle layer and its influence on the colloidal template. [1] Roth et al., Appl. Phys. Lett. 91, 091915 (2007)& Langmuir, 26, 1496 (2010) [2] Xia et al., Adv. Mat. 12, 693 (2000) [3] Koerstgens et al., Anal. Bioanal. Chem. 396, 139 (2010)

CPP 47.2 Fri 10:45 ZEU 160

Microstructures of a binary mixture of charged colloidal spheres with eutectic phase behaviour — •Thomas Palberg, Nina J. Lorenz, and Izidor Lorencak — Johannes Gutenberg Universität Mainz, Institut f. Physik, Staudingerweg 7, 55128 mainz

Using Microscopy and static light scattering we determined the phase behavior and the occurring microstructures in a binary mixture of charged colloidal spheres with a size ratio of $\Gamma = 0.57$. The eutectic point is observed at a molar fraction of small particles $x_S = 0.8$ and total number densities of about $(30 - 40)\mu m^{-3}$, which is one, resp. two orders of magnitudes larger than the freezing densities of the pure small (S) resp. large (L) particles. In the present system density and composition fluctuations needed for (heterogeneous) nucleation of coexisting S- and L-crystals are coupled to differential sedimentation. Under fluid-solid coexistence conditions we observe the majority component of small particles to form faceted crystals (at $x_S = 0.9 - 0.97$) in the bulk of the samples, while the minority component of large particles forms a network of rough, bottom wall based, hemispherical cap crystals. No faceting is observable for other mixing ratios and for the pure component systems at coexistence conditions. At number densities well above the eutectic density a correlated solidification scenario is observed, in which both species form a mosaic with intersection facets of columnar crystals growing from the container walls. Similarities and differences to morphologies observed for metallic eutectics are discussed.

CPP 47.3 Fri 11:00 ZEU 160

Influence of Pattern Height on the Dewetting of Polymer Thin Films on Topographically Patterned Substrates — •Rabibrata Mukherjee — Departmnet of Chemical Engineering, IIT Kharagpur, Pin 721302, India

Controlled dewetting of thin polymer films on physically patterned complex surfaces produces variety of ordered meso-scale structures like arrays of ordered droplets, membranes etc. In contrast to dewetting of a thin polymer film on a defect free surface, which occurs spontaneous amplification of capillary surface waves, on a topographically patterned substrate dewetting is engendered by a rapid rupture of the film along the contours of the substrate pattern. The subsequent morphological evolution is therefore strongly influenced by the geometry of the substrate pattern. We show that the final structure depends not only on a commensuration between the initial film thickness and substrate pattern geometry, but is also influenced significantly by the film preparation condition. For example, when the film is directly spin coated on to the topographically patterned substrate, the resulting morphology is strongly influenced by the height of the features, in addition to their periodicity. In contrast, when a film of uniform thickness is transferred and then dewetted on the patterned substrate, the influence of height variation of the substrate features is rather limited. In the latter case, the initial conformation of the film with respect to the underlying substrate dominates the positioning of the dewetted droplets.

CPP 47.4 Fri 11:15 ZEU 160

Heterogeneous nucleation at a flat wall in a hard sphere colloidal model system — •Markus Franke und Hans Joachim Schöpe — Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz

The hard sphere system is the simplest model system studying crystallization. Experimentally it can be realized using steric stabilized colloids. We studied the kinetics of homogeneous and wall induced heterogeneous nucleation in colloidal hard spheres as function of super saturation. Using light scattering and microscopy we can determine the time trace of the absolute crystal volume, the crystal size as well as the nucleation rate density. We show that homogeneous nucleation is mediated by precursors, while wall induced crystallization is induced by a layering at the cell wall leading to a different crystallization kinetics of wall and bulk crystals.

CPP 47.5 Fri 11:30 ZEU 160

Heterogeneous nucleation in colloids with spherical interaction — •Hans Joachim Schöpe — Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz

Understanding the process that drives a metastable liquid or fluid to the crystal state is still a challenging issue for condensed matter physics. One promising approach to the problem is offered by the study of colloidal suspensions of particles with spherical interaction. Identifying the colloidal particles as macroatoms close analogies to atomic systems are observed. Colloids offer, compared to true atomic systems, a number of advantages. On one side, the interaction potential in colloidal macroatoms can be finely controlled and tuned by the experimentalists, by engineering the properties of the particles, and/or changing the characteristics of the dispersing medium. On the other side, typical length and time scales of colloidal systems allow time-resolved observations of solidification with easily manageable experimental techniques such as microscopy and light scattering. In particular it is possible to study the competition between homogeneous and heterogeneous nucleation induced by container walls or by seeds. The results of various experiments on colloids with various interaction will be presented together with their analysis within the framework of classical theory.

CPP 47.6 Fri 11:45 ZEU 160

Nucleation in a colloidal hard sphere system using density functional theory — •Andreas Härtel[1], Martin Oettel[2], and Hartmut Löwen[1] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Germany — [2]Institut für Physik, Johannes-Gutenberg-Universität Mainz, Germany

The fluid-solid interface in a system of hard spheres is studied by density functional theory. For this purpose we employ a free minimization [1] of the White Bear II fundamental measure density functional [2] and perform a comparative study using Monte Carlo simulations [3]. Both the bulk freezing transition and the structure and thermodynamics of the hard sphere fluid-solid interface are discussed and compared to simulation data.

[1] R. Ohnesorge et al, Phys. Rev. E 50, 4801 (1994).

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

[3] M. Oettel et al, Phys. Rev. E 82, 051404 (2010).

CPP 47.7 Fri 12:00 ZEU 160

DDFT calibration and investigation of an anisotropic phase-field crystal model — •Muhammad Ajmal Choudhary[1], Daming Li[1], Heike Emmerich[1], and Löwen Hartmut[2] — [1]Lehrstuhl für Material- und Prozesssimulation, Universität Bayreuth, D-95440 Bayreuth, Germany — [2]Institut für Theoretische Physik II, Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf, Germany

The anisotropic phase field crystal (APFC) model recently proposed by Prieler et al.[J. Phys.:Condens. Matter 21, 464110 (2009)] is derived from microscopic density functional theory for anisotropic particles with fixed orientation. Further its morphology diagram is explored to demonstrate its capacity to model structures beyond those captured by the simplistic phase field crystal (SPFC) equations originally introduced by Elder et al. [Phys. Rev. Lett. 88, 245701 (2002)]. In particular we investigated the influence of anisotropy and undercooling on the process of nucleation and microstructure formation from atomic to the microscale. To that end numerical simulations were performed varying those dimensionless parameters which represent anisotropy and undercooling in our APFC model. The results from these numerical simulations are summarized in terms of a morphology diagram of the stable state phase. These stable phases are also investigated with respect to their kinetics and characteristic morphological features.

CPP 47.8 Fri 12:15 ZEU 160

Homogeneous and heterogeneous nucleation in phase field crystal models studied by the simplified string method — Rainer Backofen and •Axel Voigt — Institut für Wissenschaftliches Rechnen, TU Dresden, Dresden, Germany

The phase field crystal (PFC) model is an approximation to the classical density functional theory of liquid and solids. In recent years it has been shown that with some modification PFC gives decent descriptions of colloids or metals. We investigate a PFC model for homogeneous and heterogeneous nucleation at unstructured walls. We will show, that in order to include wall interactions the density in the classical PFC model has to be bound from below. This can be achieved by introducing a density dependent mobility or an additional density dependent potential. Thus, the wall interaction maybe tuned from wetting to non-wetting conditions. The nucleation process is analyzed directly by the Simplified String Method and the minimal stable nucleus is defined. We see that the nucleation path deviates from that one assumed in classical nucleation theory. In particular the minimal stable nucleus is not in the bulk state. Thus, the nucleation barrier is decreased.

CPP 47.9 Fri 12:30 ZEU 160

Curvature Dependence of Surface Free Energy of Liquid Drops and Bubbles — B. J. Block[1], S. K. Das[2], •M. Oettel[1,3], P. Virnau[1], and K. Binder[1] — [1]Institut für Physik, Universität Mainz, Germany — [2]Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India — [3]Material- und Prozesssimulation, Universität Bayreuth, Germany

We study the excess free energy due to phase coexistence of fluids by Monte Carlo simulations using successive umbrella sampling in finite boxes with periodic boundary conditions, allowing for stable spherical/cylindrical droplets or flat interface configurations [1]. Both the vapor-liquid phase coexistence of a simple Lennard-Jones fluid and the coexistence between A-rich and B-rich phases of a symmetric binary (AB) Lennard-Jones mixture are studied. For the surface tension $\gamma(R)$ of droplets/bubbles in the vapor-liquid case, we find for $R \to \infty$ the leading order (Tolman) correction for droplets has sign opposite to the case of bubbles, consistent with the Tolman length being independent on the sign of curvature. For the symmetric binary mixture the expected non-existence of the Tolman length is confirmed. In all cases and for a range of radii R relevant for nucleation theory, $\gamma(R)$ deviates strongly from $\gamma(\infty)$ which can be accounted for by a term of order $\gamma(\infty)/\gamma(R) - 1 \propto R^{-2}$. Comparison with density functional theory in the vapor-liquid case yields agreement in the overall behavior of $\gamma(R)$ as well as in the sign and magnitude of the Tolman length.

[1] B. J. Block, S. K. Das, M. Oettel, P. Virnau, and K. Binder, J. Chem. Phys. **133**, 154702 (2010).

CPP 48: Nanoparticles and Composite Materials II

Time: Friday 10:30–13:00 Location: ZEU 114

CPP 48.1 Fri 10:30 ZEU 114

Random nanoparticle patterns as unique optical labels for secure identification — •Alexander Schwemer[1], Ulrich Rührmair[2], and Ulrich Rant[1] — [1]Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching — [2]Institut für Informatik VI, Technische Universität München, Boltzmannstraße 3, 85748 Garching

Complex macro-structures consisting of nanoscale objects hold great potential to be used as unique labels for secure identification, because the nanoscale features render it impossible to re-produce, i.e. forge, these patterns with nm accuracy on a large scale. Here, we present a straightforward and inexpensive approach to create and read-out optical labels based on ensembles of individual metallic nanoparticles. Gold nanorods, which exhibit two plasmonic resonances with distinct spectral and polarization features, are sparsely dispersed and immobilized on a solid substrate. Light scattered from the individual particles is imaged by a dark-field microscopy setup onto a consumer-electronics grade RGB CCD camera. By recording a set of polarization dependent images we are able to deduce a specific set of parameters for each particle which encompasses the particle's position (accuracy 150 nm), its spectral properties (color), and its angular orientation on the substrate (accuracy 0.2°). We describe the experimental realization and data-analysis routines to extract an extensive set of unique data in parallel from the nano-pattern and outline the implications of the introduced concept for future use in highly sensitive security applications for valuable items such as bank notes, passports or commercial goods.

CPP 48.2 Fri 10:45 ZEU 114

New approach to low-temperature processed titania for application in inorganic-organic hybrid photovoltaics — •Monika Rawolle[1], Matthias A. Ruderer[1], Shuai Guo[1], Ezzeldin Metwalli[1], Erik V. Braden[1], Jan Perlich[2], Stephan V. Roth[2], Thomas Fröschl[3], Nicola Hüsing[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany — [2]HASYLAB at DESY, 22603 Hamburg, Germany — [3]Universität Salzburg, Materialforschung und Physik, Salzburg, Austria

Crystalline titania is a widely researched inorganic semiconductor for inorganic-organic hybrid photovoltaics. Among its many advantages are low cost and easy producibility, with the disadvantage of a necessary high-temperature step to obtain the crystalline anatase or rutile polymorph. A possible precursor for titania which does not require a high-temperature step to obtain crystallinity was previously used to create crystalline titania particles with the inverse microemulsion technique for usage in catalysis. [1] We use this precursor to prepare thin films on flexible substrates. The structure is controlled with the diblock copolymer poly(styrene-block-ethylene oxide) [P(S-b-EO)] as templating agent in a so-called good-poor solvent pair induced microphase separation combined with sol-gel chemistry. The structure of the titania films is investigated with XRR and GISAXS. Crystallinity is determined with GIWAXS for different temperatures and related to optical properties as probed with UV/Vis spectroscopy.

[1] R. Rossmanith et al., Chem. Mater. (2008) 20, 5768-5780

CPP 48.3 Fri 11:00 ZEU 114

Geordnete Nanopartikel zur Erzeugung von Höheren Harmonischen — •Valerie Mondes[1], Christina Graf[1], Jürgen Plenge[1], Qi Gao[1], Matthias Buchholz[1], Matthias Kling[2] und Eckart Rühl[1] — [1]Freie Universität Berlin, Physikalische und Theoretische Chemie, Takustr. 3, 14195 Berlin — [2]MPQ, Hans-Kopfermann-Str. 1, 85748 Garching

Neuartige Methoden zur Erzeugung Höherer Harmonischer nutzen die lokale Feldverstärkung in geordneten nanoskopischen Strukturen, indem die resonante Anregung von Plasmonen zur Feldverstärkung in Gegenwart von Edelgasen erfolgt. Es wird in dieser Arbeit die Bildung von geordneten Arrays von Nanopartikeln zur Erzeugung von kurzwelliger Strahlung genutzt. Sie bestehen aus geordneten Strukturen von isotropen und anisotropen Goldnanopartikeln, da von ihnen ausgeprägte nanoplasmonische Eigenschaften erwartet werden. Die Nanopartikel werden mit unterschiedlicher Form und Größe mit Methoden der Kolloidchemie hergestellt und durch induzierte Selbstorganisation auf Saphirträgern in Monolagen angeordnet. Die erzeugten, geordneten Nanostrukturen können damit Dimensionen bis hin zu Quadratzentimetern erreichen. Dies ist von Bedeutung, wenn durch Laserstrahlung die Strukturen beschädigt werden und stets unbeschädigte Nanostrukturen zur Erzeugung Höherer Harmonischer genutzt werden sollen. Es wurde ein Aufbau zur Detektion von kohärenten ultrakurzen XUV-Pulsen mittels eines XUV-Monochromators aufgebaut und charakterisiert. Es wird über Arbeiten zur Emission von kurzwelliger Strahlung aus den Nanostrukturen berichtet.

CPP 48.4 Fri 11:15 ZEU 114

Light induced electron spin resonance studies on films for hybrid solar cells — •Florian Witt, Marta Kruszynska, Irina Lokteva, Nikolay Radychev, Joanna Kolny-Olesiak, Holger Borchert, and Jürgen Parisi — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory (EHF), 26111 Oldenburg, Germany

Light induced electron spin resonance spectroscopy (l-ESR) is a widely used tool for the investigation of long living charges in conjugated polymers as well as in blends for organic and hybrid photovoltaics. Latter one is a synonym for solar cells out of a blend of colloidally prepared, inorganic nanocrystals and an organic conjugated polymer which act as a donor/acceptor system. With l-ESR two limiting factors in hybrid blends were investigated. At first we show the influence of traps related to unpassivated surface states on the charge carrier recombination. These states occur due to the necessary ligand exchange of the nanoparticles (A thick ligand shell resulting from colloidal synthesis needs to be replaced by smaller molecules such as pyridine to enable charge transfer). The influence of the ligand exchange treatment on the charge carrier recombination will be shown. A second focus lies on so called charge transfer complexes (CTC) in hybrid blends. These states consist of a bound polaron pair at the donor acceptor interface. We show their occurance by l-ESR.

CPP 48.5 Fri 11:30 ZEU 114

Blinking and spectral diffusion of single CdSe/ZnS colloidal nanoparticles — •Daniel Braam, Matthias Offer, Günther Prinz, Martin Geller, and Axel Lorke — Fakultät für Physik und CeNIDE, Universität Duisburg-Essen, 47048 Duisburg

Even though nanoparticles have been a main interest in research for decades, their luminecent behaviour still holds many secrets to disclose. The power-law of on- and off-times of random emission intermittency as well as several shifts in the emission wavelength still lack of a unified theory [1]. We investigated the excitonic structure of CdSe/ZnS core/shell nanoparticles using a micro-photoluminescence (μ-PL) setup with a 405 nm cw-laser. To ensure single-particle-PL we dispersed the nanoparticles in toluene with 1% PMMA and deposited these dilute solution through spin-coating on different substrates. We observed substrate-dependent emission intermittency up to nearly blinking-free emission, which we can attribute to a single CdSe nanoparticle. Spectral jumps of 25 meV in the emission can be assigned to excitonic transitions altered by a charged nanoparticle or an outer charged electronic trap state [2]. Furthermore, we observed a phonon replica of 25 meV and smaller ($<$10 meV) energetic shifts of the emission lines which are likely due to random charge variation in the surrounding of the nanoparticle.

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

[2] A. Efros, Nature Mat. **7**, 612 (2008).

CPP 48.6 Fri 11:45 ZEU 114

New Approach to Photoluminescence Intermittency: Luminescence Intensity-resolved Investigation of CdSe/ZnS Quantum Dots — •Robert Schmidt, Cornelius Krasselt, and Christian von Borczyskowski — Institute of Physics and nanoMA (Center for nanostructured Materials and Analytics), Chemnitz University of Technology, 09107 Chemnitz, Germany

The photoluminescence of single emitters like semiconductor quantum dots (QDs) shows intermittency, called blinking, which divides the intensity time traces into bright "on"-, dark "off"- and "gray" intermediate states, where the distribution of on- and off-times follow a power-law [1]. While these states can be well described by a charge separation model, the physical background of the blinking dynamics, especially of the "on"-states, is less evident. Here we investigate the fluorescence of single CdSe/ZnS-QD by single photon counting techniques and use the "change-point analysis" [2] to analyze their fluorescence time traces with respect to photoluminescence intensities. This allows us to gain new information about the "on"-state-dynamics and further insights into the fundamental physical background of QD blinking.

[1] F. Cichos, C. von Borczyskowski & M. Orrit, Current Opinion in Colloid & Interface Science **12**, 272-284 (2007).

[2] L.P. Watkins & H. Yang, J. Phys. Chem. B **109**, 617-628 (2005).

CPP 48.7 Fri 12:00 ZEU 114

Truly two-dimensional colloidal nanocrystals — •Christian Klinke — Institute of Physical Chemistry, University of Hamburg

Controlled assembly leading to anisotropic nanostructures poses a conceptual challenge in materials research. Oriented attachment of nanocrystal, a self-assembly of particles into larger single crystalline objects, is one of the most promising approaches in nanotechnology to synthesize anisotropic materials. One-dimensional assemblies of oriented attachment have been reported, and in most cases the anisotropy during self-assembly is caused by crystal planes with preferred reactivity and dipole moments in the crystallites. Systems with cubic crystal symmetry, however, like PbS and PbSe, where beautiful one-dimensional oriented attachment occurs, are somewhat more difficult to explain. In a new approach we synthesized truly two-dimensional nanocrystals by oriented attachment with lateral dimensions on the micrometer scale. We show that the formation of ordered and densely packed ligand surface layers of oleic acid on {100} PbS surfaces can drive the normally isotropic crystal growth into a two-dimensional oriented attachment of nanocrystals. Hereby the presence of chlorine containing co-solvents during the initial nucleation and growth process of the nanocrystals plays a prominent role. In the talk the synthesis and the formation mechanism will be discuss and detailed characterizations will be introduced. The obtained two-dimensional structures can be readily integrated in a photo-detector device without further treatment.

Literature: Schliehe et al., Science 329 (2010) 550.

CPP 48.8 Fri 12:15 ZEU 114

XAS and XMCD Studies on Novel Iron Oxide Nanoparticles as Magnetic Resonance Imaging (MRI) Contrast Enhancers — •Patrick Stumpf[1], Christina Graf[1], Detlef Schmitz[2], Christian Goroncy[1], Marie Küssner[1], and Eckart Rühl[1] — [1]Institut für Chemie und Biochemie - Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustr. 3, D-14195 Berlin — [2]Helmholtz-Zentrum Berlin, Albert-Einstein-Str. 15, D-12489 Berlin

Iron oxide (FeOx) nanoparticles are applied in medical research as contrast agents in magnetic resonance imaging (MRI) where they reduce the spin-spin relaxation time (T2 time) of absorbing tissue. Their magnetic properties strongly depend on the particle size and shape, as well as the surface structure and the modification of the iron oxide core. Therefore, monodisperse, spherical iron oxide (Fe3O4/Fe2O3) nanoparticles were prepared by a high temperature approach using iron oleate precursors prepared in oxygen-free and oxygen-rich surrounding. These freshly synthesized particles are tempered in an oxygen-free or oxygen-rich environment to improve their crystalline order and to change their magnetite-to-maghemite ratio. Magnetic relaxometry measurements are carried out to evaluate if these structural changes influence the spin-spin (T2) and spin-lattice (T1) relaxation times of the nanoparticles. NEXAFS (Near Edge X-Ray Absorption Fine Structure) and XMCD (X-Ray Magnetic Circular Dichroism) experiments were used to investigate local structural and electronic properties of the iron oxide particles before and after post-synthetic oxidative and thermal treatment. These results are correlated with relaxometry data.

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Synthesis, characterization, and surface functionalization of gadolinium-based nanoparticles as fluorescent and magnetic probes — •Shih-Hao Kung[1], Christina Graf[1], Christine Boeglin[2], and Eckart Rühl[1] — [1]Institut für Chemie und Biochemie, Takustr. 3, Freie Universität Berlin, 14195 Berlin, Germany — [2]Institute de Physique et Chimie des Materiaux de Strasbourg, 23, rue du Loess, BP43, F-67034 Strasbourg, France

The aim of this work is the investigation of nanoparticles which can be applied as combined fluorescent labels and T_1-weighted magnetic resonance imaging (MRI) contrast agents. Gd^{3+} with its seven unpaired electrons provides the magnetic contrast. Doping the nanoparticles with other rare earth elements, such as europium or erbium, makes the particles fluorescent. The present work is divided into two parts. The first part is a study on the magnetic properties of Gd^{3+} in the particles as well as changes when the particles are doped with fluorescent Eu^{3+}. This is achieved by X-ray magnetic circular dichroism (XMCD) measurements which were carried out at the Swiss Light Source. In the second part, results on the functionalization of nanoparticles which contain Gd^{3+} and Er^{3+} with biocompatible, hydrophilic ligands are presented. Mono- and bivalent polyethylene oxide-phosphonate ligands are prepared and the bond between the ligands and the particles are investigated by infrared spectroscopy. The ligand density is estimated by thermal gravimetric analysis. Moreover, the stability of the ligand-exchanged particles is studied by transmission electron microscopy and dynamic light scattering.

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Effective rate constants for nanostructured heterogeneous catalysts — •Shaun Hendy[1,2], Nat Lund[2], and Nicola Gaston[1,2] — [1]Industrial Research Ltd, Lower Hutt 5010, New Zealand — [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, School of Chemical and Physical Sciences, Victoria University of Wellington, Wellington 6140, New Zealand

There is currently a high level of interest in the use of nanoparticles for catalysis. With precious metal catalysts such as platinum and palladium in high demand, the use of these materials in nanoparticle form can also substantially reduce the cost of the catalyst through the exposure of more surface area for the same volume of material. When reactants are plentiful, the effective activity of a nanoparticulate catalyst will increase with its surface area, assuming that its shape is held constant and ignoring the effect of corners and edges. However, under diffusion-limited conditions, high surface area and a high density of active sites may bring diminishing returns as sites consume reactant faster than it arrives. Here we apply a mathematical homogenisation approach to derive simple expressions for the effective reactivity of a nanostructured catalyst under diffusion limited conditions that relate the intrinsic rate constants of the surfaces presented by the catalyst to an effective rate constant. When highly active catalytic sites, such as step edges or other defects are present, we show that distinct limiting cases emerge depending on the degree of overlap of the reactant depletion zone about each site. We discuss implications for the optimal design of nanoparticle catalysts.