

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

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Overview of Invited Talks and Sessions

(lecture rooms H1, H34, H39 and H40; Poster C)

Plenary and Prize Talks related to Division CPP

PV II	Mon	14:00–14:45	H1	Exploring the Functionality of Advanced Materials through Scanning Transmission Electron Microscopy — ●STEPHEN PENNYCOOK
PV VII	Tue	14:00–14:45	H15	Self-assembly, Self-organization and Control of Colloidal Suspensions — ●SABINE H. L. KLAPP
PV XII	Wed	14:00–14:45	H15	Novel Strategies for the Assembly of Quasicrystals: Epitaxial Growth of Three-dimensional Nanoporous Frameworks — ●CHRISTOF WÖLL
PV XV	Thu	13:15–13:45	H1	Near Field Optics – Science of the "Invisible Light" — ●WOLFGANG DIETER POHL
PV XVIII	Fri	8:30– 9:15	H1	Templated Self-assembly of Block Copolymer Films — ●CAROLINE ROSS

Invited Talks

CPP 1.1	Mon	9:30–10:00	H34	Rich variety of polymer dynamics in nanocomposites — ●GERALD JOHANNES SCHNEIDER
CPP 1.7	Mon	11:30–12:00	H34	Photonic structures based on responsive nanoparticle/microgel hybrids — ●THOMAS HELLWEG
CPP 2.1	Mon	9:30–10:00	H40	Langmuir monolayers as physical models in bio- and nanosciences — ●HELMUTH MÖHWALD, GERALD BREZESINSKY
CPP 5.1	Mon	15:00–15:30	H34	Intra- and inter-molecular dynamics in glass-forming liquids — ●PERIKLIS PAPADOPOULOS, WILHELM KOSSACK, FRIEDRICH KREMER
CPP 6.1	Mon	15:00–15:30	H40	a molecular picture of charge-transfer processes at donor-acceptor interfaces in organic solar cells — ●JEAN-LUC BREDAS
CPP 6.4	Mon	16:00–16:30	H40	High efficiency OLEDs based on delayed fluorescence — ●CHIHAYA ADACHI
CPP 6.7	Mon	17:00–17:30	H40	The role of intermolecular hybridization in molecular electrical doping — ●INGO SALZMANN, GEORG HEIMEL, HENRY MÉNDEZ, ANDREAS OPITZ, PATRICK BARKOWSKI, MARTIN OEHZELT, KATREIN SAUER, NORBERT KOCH
CPP 13.1	Tue	9:30–10:00	H34	Hierarchical Multi-Step Folding of Polymer Bilayers — GEORGI STOYCHEV, SEBASTIEN TURCAUD, JOHN DUNLOP, ●LEONID IONOV
CPP 16.1	Tue	9:30–10:00	H40	Functional nanolayers made from colloidal building blocks — ●ANDREAS FERY
CPP 22.1	Wed	9:30–10:00	H34	Liquid drops on soft solids — ●JACCO SNOEIJER
CPP 22.7	Wed	11:30–12:00	H34	Wetting transitions in polymer decorated nanostructured surfaces — ●JÜRGEN RÜHE
CPP 23.1	Wed	9:30–10:00	H39	Polymers, rings and pores: A neutron scattering study — ●ANDREAS WISCHNEWSKI
CPP 24.1	Wed	9:30–10:00	H40	Factors determining the contact resistance in organic thin-film transistors — MANFRED GRUBER, ●EGBERT ZOJER, FERDINAND SCHÜRRER, KARIN ZOJER
CPP 26.1	Wed	15:00–15:30	H34	Leidenfrost Dynamics — ●DAVID QUÉRÉ

CPP 28.1	Wed	15:00–15:30	H40	Self Organization of Colloidal Crystals and of Co-operative Propulsion by Salt Gradient Induced Flows — ●THOMAS PALBERG
CPP 39.1	Thu	9:30–10:00	H34	Influence of morphology on organic solar cell performance comparing crystalline diindenoperylene (DIP) and its amorphous derivative tetraphenyldibenzoperiflanthene (DBP) — STEFAN GROB, MARK GRUBER, ULRICH HÖRMANN, ●WOLFGANG BRÜTTING
CPP 40.1	Thu	9:30–10:00	H39	Collective van der Waals Interactions in Molecules, Solids, and Interfaces — ●ALEXANDRE TKATCHENKO
CPP 40.3	Thu	10:15–10:45	H39	The influence of van der Waals interactions on the adsorption of proteins to solid/liquid interfaces — ●HENDRIK HÄHL
CPP 41.1	Thu	9:30–10:00	H40	Out-of-Equilibriumness of Light Activated Colloids — ●JEREMIE PALACCI, STEFANO SACANNA, ASHER PRESKA STEINBERG, ADRIAN VATCHINSKY, KASEY HANSON, DAVID PINE, PAUL CHAIKIN
CPP 41.4	Thu	10:30–11:00	H40	Mesoscale Simulations of Active Colloids — ●GERHARD GOMPPER
CPP 41.8	Thu	12:00–12:30	H40	Orientalional Order and Packings of Non-Spherical Particles — ●KLAUS MECKE, RENE WITTMANN, SEBASTIAN KAPFER, GERD SCHRÖDER-TURK
CPP 43.1	Thu	15:00–15:30	H34	Quantum coherence controls the charge separation in a prototypical artificial light harvesting system — ●C. LIENAU, S. M. FALKE, C. A. ROZZI, N. SPALLANZANI, A. RUBIO, E. MOLINARI, D. BRIDA, M. MAIURI, G. CERULLO, H. SCHRAMM, J. CHRISTOFFERS
CPP 44.1	Thu	15:00–15:30	H39	Dynamic reorganization of droplets: from Foams to Phonons — ●RALF SEEMANN, JEAN-BAPTISTE FLEURY, ULF D. SCHILLER, SHASHI THUTUPALLI, OHLE CLAUSSEN, STEPHAN HERMINGHAUS, GERHARD GOMPPER, MARTIN BRINKMANN
CPP 44.7	Thu	17:00–17:30	H39	Wetting behaviour in inkjet printed droplets — ●PATRICK SMITH, JONATHAN STRINGER
CPP 45.1	Thu	15:00–15:30	H40	Interacing colloidal fluids self-assembled from supramolecular polymers — TINGZI YAN, KLAUS SCHRÖTER, FLORIAN HERBST, WOLFGANG BINDER, ●THOMAS THURN-ALBRECHT
CPP 47.1	Fri	9:30–10:00	H34	Ion transport in polyelectrolyte materials: Mechanisms and general scaling concepts — ●MONIKA SCHÖNHOF, CORNELIA CRAMER, SOUVIK DE, AMRTHA BHIDE
CPP 48.1	Fri	9:30–10:00	H39	The distribution of segmental order in polymer networks — ●MICHAEL LANG, JENS-UWE SOMMER
CPP 49.1	Fri	9:30–10:00	H40	Interface-controlled property adjustment in ionic liquid/inorganic hybrid materials — ●ANDREAS TAUBERT

Symposium Charge Transfer Effects in Molecular Materials (SYCT)

SYCT 1.1	Mon	9:30–10:00	H1	A coarse grained QM/MM approach for the description of charge transfer in complex systems — ●MARCUS ELSTNER
SYCT 1.2	Mon	10:00–10:30	H1	Identifying and resolving charge separation in organic solar cells — ●EBERHARD RIEDLE
SYCT 1.3	Mon	10:30–11:00	H1	Quantifying the energy of charge transfer states: From molecular crystals to donor-acceptor blends — ●REINHARD SCHOLZ
SYCT 1.4	Mon	11:00–11:30	H1	Efficient Exciton Generation and Collection in Organic Solar Cells — ●MARK THOMPSON, CONG TRINH, STEVE FORREST, JEREMY ZIMMERMAN
SYCT 1.5	Mon	11:30–12:00	H1	Electron transport in organic single-crystal transistors and Schottky-gated heterostructures — ●ALBERTO MORPURGO

Symposium Quantum Plasmonics (SYBD)

SYBD 1.1	Mon	15:00–15:30	H1	Functionalization and Pharmaceutical Aspects of Magnetic Nanoparticles (Magnetic Carriers) — ●URS O. HÄFELI
SYBD 1.2	Mon	15:30–16:00	H1	Fluid mechanical aspects of therapeutic application of suspensions of magnetic nanoparticles — ●STEFAN ODENBACH
SYBD 1.3	Mon	16:00–16:30	H1	Magnetic Particle Imaging: A new Medical Imaging Modality — ●THORSTEN BUZUG

SYBD 1.4	Mon	16:30–17:00	H1	Superparamagnetic iron oxide nanoparticles for MR-visible mesh implants and novel drug targeting models — ●IOANA SLABU, ANJALI ROETH, CHRISTIANE KUHLE, THOMAS SCHMITZ-RODE, MARTIN BAUMANN
SYBD 1.5	Mon	17:00–17:30	H1	Magnetic measurement techniques assisting biomedical applications of magnetic nanoparticles — ●LUTZ TRAHMS

Symposium Magnetic Nanoparticles in Biomedical Diagnostics and Therapy (SYMM)

SYMM 1.1	Thu	9:30–10:00	H1	Challenges for first-principles based computation of properties of oxide materials — ●KARSTEN ALBE
SYMM 1.2	Thu	10:00–10:30	H1	Deformation and Fracture of Solids: Tough Nuts at Atomic and Continuum Scales — ●PETER GUMBSCH, MATOUS MROVEC, KINSHUK SRIVASTAVA, DANIEL WEYGAND
SYMM 1.3	Thu	10:30–11:00	H1	Crucial Issues and Future Directions of Through-Process Modeling — ●GUENTER GOTTSTEIN
SYMM 1.4	Thu	11:00–11:30	H1	Adaptive Resolution Simulations for Soft Matter: Applications and New Developments — ●KURT KREMER
SYMM 1.5	Thu	11:30–12:00	H1	Materials by design — ●MARKUS BUEHLER

Sessions

CPP 1.1–1.13	Mon	9:30–13:30	H34	Nanoparticles and Composite Materials I
CPP 2.1–2.14	Mon	9:30–13:30	H40	Interfaces and Thin Films I (joint session with DECHEMA and VDI)
CPP 3.1–3.5	Mon	12:15–13:30	H1	Charge Transfer Effects in Molecular Materials I (joint session CPP/HL/BP/DS)
CPP 4.1–4.5	Mon	15:00–17:30	H1	SYBD: Magnetic Nanoparticles in Biomedical Diagnostics and Therapy
CPP 5.1–5.9	Mon	15:00–17:30	H34	Glasses and Glass Transition I (joint session DY/CPP)
CPP 6.1–6.7	Mon	15:00–17:30	H40	Charge Transfer Effects in Molecular Materials II (joint session CPP/HL/BP/DS)
CPP 7.1–7.6	Mon	17:15–18:45	H32	Organic Electronics and Photovoltaics I (joint session DS/CPP/HL/O)
CPP 8.1–8.16	Mon	17:30–19:30	Poster C	Poster: New Instruments and Methods
CPP 9.1–9.42	Mon	17:30–19:30	Poster C	Poster: Interfaces and Thin Films (joint session with DECHEMA and VDI)
CPP 10.1–10.8	Mon	17:30–19:30	Poster C	Poster: Charge transfer effects in molecular materials (related to symposium SYCT)
CPP 11.1–11.15	Mon	17:30–19:30	Poster C	Poster: Glasses and Glass Transition (joint session DY/CPP)
CPP 12.1–12.32	Mon	17:30–19:30	Poster C	Poster: Nanoparticles and Composite Materials
CPP 13.1–13.12	Tue	9:30–13:00	H34	Biomaterials and Biopolymers I (joint session CPP/BP)
CPP 14.1–14.13	Tue	9:30–13:00	H39	Crystallization, Nucleation and Self Assembly I
CPP 15.1–15.12	Tue	9:30–12:45	H32	Organic Electronics and Photovoltaics II (joint session DS/CPP/HL/O)
CPP 16.1–16.12	Tue	9:30–13:00	H40	Interfaces and Thin Films II (joint session with DECHEMA and VDI)
CPP 17.1–17.11	Tue	9:30–12:30	H46	Glasses II (joint session DY/DF/CPP)
CPP 18.1–18.24	Tue	18:15–20:15	Poster C	Poster: Polymer Dynamics
CPP 19.1–19.11	Tue	18:15–20:15	Poster C	Poster: Crystallization, Nucleation and Self Assembly
CPP 20.1–20.36	Tue	18:15–20:15	Poster C	Poster: Colloids and Complex Liquids
CPP 21.1–21.12	Wed	9:30–12:45	H2	Transport: Molecular Electronics (joint session TT/CPP/HL/MA)
CPP 22.1–22.11	Wed	9:30–13:00	H34	Focus: Wetting on smooth and rough surfaces: From spreading to superhydrophobicity I
CPP 23.1–23.12	Wed	9:30–13:00	H39	Polymer Dynamics
CPP 24.1–24.12	Wed	9:30–13:00	H40	Organic Semiconductors
CPP 25.1–25.11	Wed	9:30–12:45	H43	Biomaterials and Biopolymers II (joint session BP/CPP)
CPP 26.1–26.5	Wed	15:00–16:30	H34	Focus: Wetting on smooth and rough surfaces: From spreading to superhydrophobicity II

CPP 27.1–27.6	Wed	15:00–16:30	H39	Nanoparticles and Composite Materials II
CPP 28.1–28.5	Wed	15:00–16:30	H40	Crystallization, Nucleation and Self Assembly II
CPP 29.1–29.12	Wed	16:00–19:00	H33	Organic Electronics and Photovoltaics III (joint session O/CPP/DS/HL)
CPP 30.1–30.14	Wed	16:30–18:30	Poster C	Poster: Focus: Wetting on smooth and rough surfaces: From spreading to superhydrophobicity
CPP 31.1–31.22	Wed	16:30–18:30	Poster C	Poster: Organic Electronics and Photovoltaics (joint session DS/HL/O/CPP)
CPP 32.1–32.15	Wed	16:30–18:30	Poster C	Poster: Organic Semiconductors
CPP 33.1–33.15	Wed	16:30–18:30	Poster C	Poster: Charged Soft Matter
CPP 34.1–34.23	Wed	16:30–18:30	Poster C	Poster: Wetting, Micro and Nano Fluidics
CPP 35.1–35.5	Wed	16:30–18:30	Poster C	Poster: Biomaterials and Biopolymers (joint session BP/CPP)
CPP 36.1–36.8	Wed	16:30–18:30	Poster C	Poster: (Hydro)gels and Elastomers
CPP 37.1–37.2	Wed	16:30–18:30	Poster C	Poster: Focus: Van der Waals at soft matter interfaces: structure and dynamics
CPP 38.1–38.5	Thu	9:30–12:00	H1	SYMM: Computational Challenges in Scale-Bridging Modeling of Materials
CPP 39.1–39.12	Thu	9:30–13:00	H34	Organic Electronics and Photovoltaics IV (joint session CPP/HL/O/DS)
CPP 40.1–40.5	Thu	9:30–11:15	H39	Focus: Van der Waals at soft matter interfaces: structure and dynamics
CPP 41.1–41.10	Thu	9:30–13:00	H40	Colloids and Complex Liquids I
CPP 42.1–42.6	Thu	11:30–13:00	H39	New Instruments and Methods
CPP 43.1–43.13	Thu	15:00–18:45	H34	Organic Electronics and Photovoltaics V (joint session CPP/HL/O/DS)
CPP 44.1–44.12	Thu	15:00–18:45	H39	Wetting, Micro- and Nanofluidics
CPP 45.1–45.13	Thu	15:00–18:45	H40	Colloids and Complex Liquids II
CPP 46.1–46.17	Fri	9:15–13:45	H2	Photovoltaics (joint session HL/CPP/O)
CPP 47.1–47.9	Fri	9:30–12:00	H34	Charged Soft Matter
CPP 48.1–48.9	Fri	9:30–12:00	H39	(Hydro)gels and Elastomers
CPP 49.1–49.9	Fri	9:30–12:00	H40	Colloids and Complex Liquids III

Annual General Meeting of the Chemical and Polymer Physics Division

Wednesday 19:00–20:00 H34

- Report
- Discussion about DPG Fellows
- Conference 2014 (suggestions for symposia and focus sessions?)
- CPP Poster prize
- Other topics

Annual Meeting of the DECHEMA and VDI ProcessNet “Grenzflächenbestimmte Systeme und Prozesse”

Monday 19:00–20:00 PHY 5.0.21

CPP 1: Nanoparticles and Composite Materials I

Time: Monday 9:30–13:30

Location: H34

Invited Talk

CPP 1.1 Mon 9:30 H34

Rich variety of polymer dynamics in nanocomposites — ●GERALD JOHANNES SCHNEIDER — Jülich Centre for Neutron Science, Forschungszentrum Jülich, Outstation at FRM2, Lichtenbergstraße 1, 85747 Garching

Nanocomposites show prominent features in comparison with their respective ingredients. These manifest themselves in a broad range of applications ranging from reinforced rubber to energy related devices. Despite their importance, the respective molecular mechanisms are very complex and remain poorly understood. Particularly this is the case, when attractive interactions of the chains with the surfaces are involved, and e.g. immobilization of chains within an adsorbed layer in the close vicinity of the particles is expected.

In a step toward a better understanding of nanocomposites, the talk illuminates the microscopic polymer dynamics exploiting the high spatial and time resolution of neutron scattering experiments. Using neutron spin echo and time-of-flight spectroscopy, a broad dynamic range – from the segmental relaxation up to the center of mass diffusion of the polymer chains – is explored. This allows for an accurate and detailed picture of the influence of the interaction strength on the chain dynamics and in particular on the molecular motion within the interphase, i.e. in the small layer of adsorbed chains.

CPP 1.2 Mon 10:00 H34

Investigation of particle-induced confinement effects on free volume in PEP-Silica Nanocomposites — ●CHRISTIAN OHRT¹, TÖNJES KOSCHINE¹, STEPHAN HARMS¹, KLAUS RÄTZKE¹, FRANZ FAUPEL¹, LUTZ WILLNER², and GERALD SCHNEIDER³ — ¹Materialwissenschaft-Materialverbunde, Universität Kiel, 24143 Kiel — ²Jülich Centre for Neutron Science 1 and Institut für Complex Systems Forschungszentrum Jülich, D-52425 Jülich — ³Forschungs-Neutronenquelle Heinz Maier-Leibnitz 85747 Garching Germany

PPolymer nanocomposites are widely used due to improved properties compared to pure polymers. Some of the improved properties can be a result of a so called interphase, a part with a modified free volume, resulting from the interaction between nanoparticles and polymer or they can be a consequence of the restricted mobility of polymer chains due to the nanoparticles, usually termed confinement. Positron annihilation lifetime spectroscopy (PALS) can be used to investigate the influence of nanoparticles in a polymer matrix on the free volume. We analysed the change in free volume due to confinement in a weakly repulsive system consisting of poly(ethylene-alt-propylene) (PEP) with different molecular weights and silica nanoparticle concentrations by PALS and thermal properties by DSC. DSC showed no change in glass transition temperature, whereas PALS showed an increase in o-Ps lifetimes for low temperatures and a decrease for high temperatures with increasing filler concentration, which can be explained by a mixing rule of o-Ps lifetimes of the pure constituents. Thus no interphase is formed and the dynamics of the polymer are not affected by confinement.

CPP 1.3 Mon 10:15 H34

An unusual viscosity behaviour of the nanocomposites — ●MARTA LUNGOVA, WIM PYCKHOUT-HINTZEN, and DIETER RICHTER — Forschungszentrum Jülich, Germany

Many polymers have been modified by adding the suitable nanoparticles resulting in a higher modulus and viscosity. However, some systems showed the opposite effect [1]. The reduced viscosity was also observed on the system of linear PEO with PEO-grafted silica nanoparticles where in a similar way, the size of the nanoparticles is in the range of the tube diameter of the bulk polymer. The viscosity reduction becomes more evident with increasing Mw but crosses-over to the opposite, reinforcement effect, for high Mw of the matrix. This is apparently a function of the ratio between the radius of the nanoparticle and the Rg of the bulk polymer.

The SANS experiment (ILL, France and FRM II, Germany) showed that the polymer shell of the nanoparticle tends to be more swollen in the matrix of low Mw whereas with increasing Mw of the bulk the shell collapses and particles separate from the matrix resembling rigid particles with the typical reinforcement effect. The dynamics of the bulk polymer measured by NSE (ORNL, USA) were slowed down in a system with higher viscosity.

This work is a part of the European project DYNACOP supported

by Marie Curie Action.

[1] Mackay M. et al, Nat.Mater., 2003, 762-6.

CPP 1.4 Mon 10:30 H34

Structural investigation of polymer-metal nanocomposite films using time-of-flight grazing incidence small angle neutron scattering — ●YUAN YAO¹, EZZELDIN METWALLI¹, JEAN-FRANCOIS MOULIN², MARTIN HAESE-SELLER², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — ²HZ Geesthacht at FRM II, Lichtenbergstr.1, 85748 Garching, Germany

Soft polymer films with embedded magnetic nanoparticles have attracted immense interest for wide potential applications in functional nano-devices. Well-aligned highly-oriented hybrid films of polystyrene(deuterated)-block-polybutyl methacrylate symmetric block copolymer are used to guide polystyrene grafted maghemite nanoparticles within the polymer matrix. Parallel and perpendicular lamella structured films, embedded with different nanoparticles concentrations (from 0 up to 15 wt%), are prepared by spin coating process. Both surface and buried structural information of the metal-polymer hybrid film are gained using TOF-GISANS. The nanoparticles are positioned in one polymer domain and a distortion of the lamella structure evolves with increasing nanoparticle concentration. The nanoparticles arrangement and possible particle assemblies within the polymer matrix is influenced by the lamella orientation.

CPP 1.5 Mon 10:45 H34

Structure and morphology of hybrid thin films for non-volatile memories — ●JIRÍ NOVÁK¹, GIULIA CASULA², RUPAK BANERJEE¹, CHRISTIAN FRANK¹, ALEXANDER GERLACH¹, KATHARINA BROCH¹, PIERO COSSEDDU², ANNALISA BONFIGLIO², and FRANK SCHREIBER¹ — ¹Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen — ²University of Cagliari, DIEE, Piazza d'Armi, 09123 Cagliari, Italy

Recently, hybrid thin films comprising metal nanoparticles (NPs) embedded in an organic semiconductor (OSM) matrix became attractive as constituents of non-volatile resistive memories [1,2]. The control of the structure of hybrid films via growth parameters is of crucial interest to tailor the electric properties of the memory elements.

We present a structural study on the formation of Al NPs atop thin organic films (small molecule OSM N1400 by Polyera). The films were prepared via thermal evaporation on Si substrates for various organic film thicknesses and at various Al growth rates. The combined GISAXS, X-ray reflectivity, and AFM study shows that the Al cluster distance and size depend mainly on the organic layer morphology controlled by its thickness. On the other hand, the Al NPs layer structure is weakly sensitive to the Al deposition rate. This is in a strong contrast to, e.g., growth of Au on top of DIP layers, where rather Au growth rate and substrate temperature play a crucial role [3].

[1] L.D. Bozano *et al.*, *Adv. Funct. Mater.*, **15**, 1993 (2005); [2] Liping Ma *et al.*, *Appl. Phys. Lett.*, **82**, 1419 (2003); [3] F. Schreiber, *Phys. Stat. Sol.*, **201**, 1307 (2004);

CPP 1.6 Mon 11:00 H34

In situ SAXS measurements on the imbibition of polymer melts into aligned CNT arrays — ●MARINA KHANEFT¹, LUCAS BECKER¹, THORSTEN HEINLEIN², HERMANN TEMPEL², JÖRG J. SCHNEIDER², and BERND STÜHN¹ — ¹Experimentelle Physik kondensierter Materie, Technische Universität Darmstadt — ²Eduard Zintl-Institute für Anorganische und Physikalische Chemie Technische Universität Darmstadt

We present results on the imbibition of the polymer into aligned carbon nanotube (CNT) arrays and describe the filling kinetics of the polymer. The aligned CNT structures were prepared by CVD method. We considered two types of CNT arrays: well ordered CNTs prepared within porous alumina template (PAOX). CNTs have a diameter around 40 nm and are arranged on a hexagonal lattice as were the pores of PAOX template. A second kind of CNT array consists of randomly arranged tubes with small diameter (<10 nm) grown on a quartz surface by catalytic CVD approach. The imbibitions process of polystyrene (PS) into the CNT array is followed with time-resolved small angle X-ray scattering (SAXS). We observed polymer infiltration into tube inte-

rior and interstices between CNTs. For CNT array grown in PAOX template, filling kinetics inside and outside tubes can be analysed separately. Infiltration only in inner part of CNTs can be achieved by polymer filling of CNTs situated in PAOX. Interstices between tubes can be filled after removing the template. We found the filling kinetics demonstrates two well separated processes: the formation of a precursor film and completion of the imbibition process.

15 min. break

Invited Talk CPP 1.7 Mon 11:30 H34
Photonic structures based on responsive nanoparticle/microgel hybrids — ●THOMAS HELLWEG — Universität Bielefeld, Physikalische und Biophysikalische Chemie (PC III), Universitätsstr. 25, 33615 Bielefeld, Germany

Microgels based on responsive polymers can be combined with metal nanoparticles leading to materials with responsive optical properties (1). Ordering of nanoparticles into assemblies which are well-defined on the nanoscale and at the same time of macroscopic dimensions is one of the most pressing challenges in materials science. If particles are aggregating in a random fashion, often uncontrolled electronic coupling effects occur, which result in less defined electronic, optical or magnetic properties or in a complete loss of the specific nanoparticle effects and a re-entrance of bulk material properties. Creating ordered nanoparticle structures is one means of avoiding such uncontrolled coupling. In this context hybrids of microgels and nanoparticles are offering interesting pathways for 2 and 3 D assembly (2,3). The present contribution will describe the properties of these hybrids and discuss strategies of their assembly.

- (1) Karg, M. und T. Hellweg, *Current Opinion in Coll. Interf. Sci.*; 14, 438–450, 2009
- (2) Müller, M., M. Karg, A. Fortini, T. Hellweg und A. Fery, *Nanoscale*, 4:2491–2499, 2012
- (3) Karg, M., T. Hellweg und P. Mulvaney, *Adv. Func. Mater.*; 21:4668–4676, 2011

CPP 1.8 Mon 12:00 H34
Photoinduced phase transitions in gold-microgel hybrids — ●SARAH T. TURNER, STEFAN WELLERT, and REGINE VON KLITZING — Stranski Laboratory, Dept. of Chemistry, TU Berlin, Germany

The ability to reversibly switch between a collapsed and expanded state in response to an external stimulus makes hybrid microgels attractive for applications such as sensoric and drug delivery systems. We studied the photoinduced light-to-heat conversion and consequent volume phase transition of hybrid gold-microgels. In order to use such hybrid systems as a potential barrier in polyelectrolyte multilayers, details about the degree of shrinking related to the gold loading and laser intensity are required. An optimal gold nanoparticle concentration per microgel was found to exist, as too low a concentration does not allow enough heat formation to induce a volume phase transition and too high a concentration hinders the full swelling of the microgel below the lower critical solution temperature. The distribution and loading of the gold nanoparticles is investigated via transmission electron microscopy and the change in the plasmon resonance of the gold nanoparticles upon microgel shrinking is investigated by temperature-controlled UV-Vis absorption spectroscopy. The plasmon resonance frequency of the gold nanoparticles was excited by one laser (532 nm) while a second was used to simultaneously measure dynamic light scattering (633 nm) by blocking the scattering signal from the first laser with an optical filter.

CPP 1.9 Mon 12:15 H34
Wrinkle-Assisted Self-Assembly of PNIPAM Coated Nanostars as SERS Platforms for Sensing of PAHs in Gas Phase — MAREEN MUELLER, ●MORITZ TEBBE, NICOLAS PAZOS-PEREZ, and ANDREAS FERY — Department of Physical Chemistry II, University of Bayreuth, 95440, Bayreuth, Germany

Plasmonic nanoparticles are excellent candidates for their potential use in microelectronic, optical and biomedical applications. Their electromagnetic behaviour is highly dependent on their specific particle size, shape, and surrounding environment. Various different synthetic methods allow us to fine tune the particle shape and size thus, the materials properties. However, the lack of capability to form reproducible organized structures is still a challenge to solve in order to use them in new technologies. Template-assisted self-assembly is a versatile platform to generate particle assemblies in high quality and with high reproducibil-

ity. Compared to lithographically prepared templates, controlled surface wrinkling on elastomers is an alternative approach to produce structured surfaces with periodicities in the range of nanometres. The use of wrinkled surfaces as templates for nanoparticle alignment via printing, results in highly ordered nanoparticle arrays. In this work a new surface enhanced Raman spectroscopy (SERS) platform based on the extended organization of poly-N-isopropylacrylamide (pNIPAM)-coated gold nanostars over large areas into parallel lines is presented.[1] This system yields high and homogeneous SERS intensities, and simultaneously traps PAH traces, e.g. pyrene, as pollutants from the gas phase. 1. Mueller, M., et al., *Langmuir*, 2012. 28(24): p. 9168-9173.

CPP 1.10 Mon 12:30 H34
effective interactions in polymer-nanoparticle composites and their resulted phase structures — ●XUEZHENG CAO¹, HOLGER MERLITZ^{1,2}, and JENS UWE SOMMER^{1,3} — ¹Leibniz Institute für Polymerforschung Dresden, D-01069 Dresden, Germany — ²Department of Physics and ITPA, Xiamen University, Xiamen361005, P.R.China — ³Technische Universität Dresden, Institute of Theoretical Physics, D-01069 Dresden

We have studied polymer induced effective interactions between nanoparticle-nanoparticle and nanoparticle-substrate using molecular dynamics simulations. To analyze the entropic depletion potential, the polymer matrix above overlap concentration is regarded as a melt of concentration blobs. Convincing numerical evidence for the universal validity of scaling theory to describe the depletion potentials over a broad concentration range was found, and the directly measured depletion forces were well described with a scaling model in which the attraction between particles is caused by the depletion of concentration blobs. Adding enthalpic attraction between polymer-nanoparticle or polymer-nanoparticle can prevent the depletion effect. A thermodynamically stable dispersion of nanoparticles within polymer solution is verified to be possible by tuning the attraction strength between polymer and nanoparticle. We show that nanoparticles have a higher degree of order close to the substrate by increasing system temperature. This can be understood by scaling arguments showing the interplay between correlation blob and adsorption blob of polymers.

CPP 1.11 Mon 12:45 H34
Conformational Transitions in Polymer Brushes — ●DIRK ROMEIS^{1,2} and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden, Germany — ²Technische Universität Dresden, Germany

Due the large density gradients in polymer brushes strong interaction forces are present leading to stretched chain conformations with the end-to-end distance scaling linearly with the degree of polymerization. In such an environment slight modifications of individual brush chains have great effects on their conformations [1,2]. We developed a quasi off-lattice SCF Model, that accounts for finite extensible polymer chains composed of differently sized and interacting spherical monomers. It allows for a realistic description of polymer brushes up to high grafting densities and the results are in excellent agreement to corresponding MD simulation [3], including packing, fluctuation and depletion effects. Using this approach we analyzed the behavior of individually modified guest chains in polymer brushes and encountered conformational transitions revealing a scaling behavior that can be rationalized using an analytical model. [1] Merlitz H. et. al. [*Macromolecules* **41** 5070, 2008] [2] Merlitz H. et. al. [*PRL* **102** 115702, 2009] [3] Romeis D. et. al. [*JCP* **136** 044903, 2012]

CPP 1.12 Mon 13:00 H34
Thermally stable composites of block-copolymer/metal nanoparticles. — ●IRYNA PEREPICHKA, DMITRII PEREPICHKA, and BRUCE LENNOX — Department of Chemistry, McGill University, Montreal (QC) Canada

Metal nanoparticles are widely studied for their applications in medicine, cosmetics, sensing, data storage, etc. Use of nanoparticles as catalysts in organic synthesis is another promising direction. However, many reactions require high temperatures, at which most nanoparticles solutions are unstable. Thus, producing metal nanoparticles that would not agglomerate during organic reaction is challenging.

We have synthesized gold and copper nanoparticles that are stable at above 150 C in various organic solvents. Role of ligands in nanoparticles stabilization has been studied. We have shown that combination of metal nanoparticles and diblock copolymers results in stable nanoformulations. Use of thus prepared Cu and Au NP as catalysts for aromatic C-C coupling reactions will be discussed.

CPP 1.13 Mon 13:15 H34

Charge transfer and recombination in hybrid solar cells with CuInS₂ nanocrystals studied by light-induced electron spin resonance — ●CHRISTOPHER KRAUSE, RANY MIRANTI, DOROTHEA SCHEUNEMANN, FLORIAN WITT, JOANNA KOLNY-OLESIK, HOLGER BORCHERT, and JÜRGEN PARISI — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, 26129 Oldenburg

Organic-inorganic hybrid solar cells made of semiconductor nanocrystals embedded into an organic material have made considerable progress in recent years. The highest efficiencies of such kind of solar cell are currently reached with cadmium based semiconductor nanoparticles, which have the drawback of a high toxicity. Therefore

we investigate the application of CuInS₂ nanoparticles as a promising new candidate for organic-inorganic hybrid solar cells. By ligand exchange procedures we are able to modify the surface of the nanoparticles in order to enable an efficient charge transfer and control the number of trap states arising from dangling bonds. In this contribution, light-induced electron spin resonance (LESER) measurements on composites of CuInS₂ nanoparticles with P3HT and PCBM will be presented. LESER is used to study the charge transfer at the hybrid donor/acceptor interface and its dependence on the ligand shell. Besides proving a successful photo-induced charge transfer we can use this method to investigate the density of trap states by analyzing the recombination kinetics of photo-generated long-lived charge carriers at different temperatures.

CPP 2: Interfaces and Thin Films I (joint session with DECHEMA and VDI)

The session is a joint session with ProcessNet "Grenzflächenbestimmte Systeme und Prozesse" of DECHEMA and VDI.

Organizers: Thomas Danner (BASF), Leo Nick (DECHEMA) and Regine v. Klitzing.

Time: Monday 9:30–13:30

Location: H40

Invited Talk

CPP 2.1 Mon 9:30 H40

Langmuir monolayers as physical models in bio- and nanosciences — ●HELMUTH MÖHWALD and GERALD BREZESINSKY — Max-Planck-Inst.of Colloids and Interfaces, 14424 Potsdam

Monolayers of amphiphilic molecules on water surfaces are on one hand excellent models to study ordering processes in 2 dimensions on a flexible and amorphous substrate, on the other hand they may serve as biophysical models to study processes at membrane surfaces. A plethora of techniques has been developed in the past to study the films in detail, the most important ones X-Ray diffraction, reflection and fluorescence and FTIR spectroscopy. - Polyoxometallates as most defined inorganic clusters with high application potential in catalysis and optics can be coupled with hydrocarbon chains, and ordering of the system at an interface is physically interesting in view of the competitive interactions of the clusters and the chains. - Peptides can arrange at interfaces leading to changes of secondary structures. These can be modeled theoretically including their additionally interactions with ions. one can thus contribute to processes that are involved in various diseases like Alzheimer's. - Sugars are important for recognition processes in biology, and many of these processes occur at membrane surfaces. Thus studies of their arrangement at interfaces are most welcome. It will be shown that they can form a strong crystalline hydrogen bonded network, and if these molecules are coupled to aliphatic chains the competition between chain and sugar ordering can be won by the latter. the resulting structure is again in agreement with molecular dynamics simulations.

CPP 2.2 Mon 10:00 H40

The influence of compressed gases on lipid monolayers — FRIEDERIKE GIEBEL, ●JULIA NASE, MICHAEL PAULUS, STEFFEN BIEDER, IRENA KIESEL, and METIN TOLAN — Fakultät Physik/DELTA, TU Dortmund, 44221, Dortmund, Germany

An intact cell membrane is essential for the correct functionality of cells in the human body. Depending on their solubility and size, gas molecules can cross the cell barrier by diffusion through the membrane. Thus, the question of how diverse harmful substances can modify membranes is of eminent importance for the understanding of basic mechanisms of malfunctions. To reduce the complexity of the bilayer and gain access to more basic mechanisms, simple lipid monolayers are a well-established model system. These so-called Langmuir layers are formed at the water-gas interface if certain lipids are applied carefully to the water surface.

We investigated the influence of diverse pressurized gases on the structure of a lipid monolayer using high-energy synchrotron radiation at ID10 of ESRF. The vertical structure of the interface was determined via x-ray reflectivity measurements, whereas changes in the lateral structure were detected from GID measurements. We observed an adsorption of gas molecules on the lipid layer. A change in the film structure was evident in the presence of gas, and the Langmuir film remained stable.

CPP 2.3 Mon 10:15 H40

Protein Adsorption at the Electrified Air-Water Interface: Implications on Foam Stability

— ●BJÖRN BRAUNSCHWEIG, KATHRIN ENGELHARDT, and WOLFGANG PEUKERT — University of Erlangen-Nuremberg, Institute of Particle Technology (LFG), Germany

The interfacial structure of ions, water molecules and surface active proteins as well as their tendency to form foam stabilizing networks can considerably influence and control macroscopic properties of foamy dairy products. The molecular structure and composition of adjacent electric double layers are, however, not yet fully understood on a molecular level. We have applied vibrational sum-frequency generation (SFG) as an inherently interfacial specific probe that provides information on composition and conformation of interfacial layers. In particular, we have addressed the adsorption of bovine serum albumin (BSA) at air-water interfaces and show pH depending charging and electric field-induced polar ordering of interfacial molecules such as H₂O and BSA. Varying the bulk pH of protein dilutions, changes the SFG intensity of vibrational bands due to interfacial H₂O dramatically while much weaker changes in the protein related Amide I and carboxylate R-COO⁻ bands are observed. Using the intensity of OH vibrational bands as a measure of the interfacial electric field, we have determined the isoelectric point of interfacial BSA. Based on the molecular level information from our SFG and ellipsometric measurements we can link the microscopic properties of BSA at the air-water interface with macroscopic properties such as the stability of BSA foams.

CPP 2.4 Mon 10:30 H40

Nanoparticle-induced permeability of lipid bilayer membranes — SERGEY POGODIN¹, ●MARCO WERNER^{2,3}, JENS-UWE SOMMER^{2,3}, and VLADIMIR A. BAULIN^{4,5} — ¹Institut Català d'Investigació Química, Tarragona, Spain — ²Leibniz-Institut für Polymerforschung Dresden, Germany — ³Technische Universität Dresden, Germany — ⁴Universitat Rovira i Virgili, Tarragona, Spain — ⁵ICREA, Barcelona, Spain

Using lattice Monte Carlo simulations with explicit solvent we investigate interactions of nanoparticles with self-assembled bilayer membranes as function of nanoparticle hydrophobicity and heterogeneity of amphiphilic site distribution. Our simulation results indicate, that there is an adsorption transition for nanoparticles at the model membrane for intermediate values of nanoparticle hydrophobicity, where the effective repulsions from solvent- and lipid tail environments are balanced. Close to this transition, we observe a significant frequency increase of nanoparticle translocations through the bilayer as well as an increased bilayer permeability for solvent. Depending on nanoparticle concentration we observe clustering of homogeneous nanoparticles to larger agglomerates perturbing the membrane on a larger scale. Amphiphilic nanoparticles as used in our study do not agglomerate and show an enhanced localization at the bilayer surface as compared to homogeneous nanoparticles.

CPP 2.5 Mon 10:45 H40

Messung des Transfermassenstroms nanoskaliger Partikeln

über die Grenzfläche gegensätzlich polarer Flüssigkeiten — ●PHILIPP GRIMM¹, JACQUELINE ERLER², URS A. PEUKER² und HANS-JOACHIM SCHMID¹ — ¹Universität Paderborn — ²TU Bergakademie Freiberg

Nanoskalige Organosole werden häufig als Nanokomposite oder im Bereich der Beschichtungstechnologie eingesetzt. Die Synthese der Partikeln findet üblicherweise in wässriger Umgebung statt, was jedoch zu Agglomeration und somit zum Verlust der spezifischen Eigenschaften (z.B. Superparamagnetismus) führt.

Als Transferapparat kommt hierbei eine Einzeltropfensäule zum Einsatz. Das Hauptaugenmerk liegt darin, den Transfermassenstrom in Abhängigkeit der Parameter Grenzflächengröße, Verweilzeit und Tensid- zu Partikelmasse messtechnisch zu erfassen.

Hierzu wird ein neuartiger Aufbau vorgestellt, der die Messung der relevanten Größen mittels Röntgenabsorption ermöglicht. Dieses ist notwendig, da das Stoffsystem bedingt durch Streuung keine optische Zugänglichkeit der Tropfeneigenschaften bietet. Die Röntgenstrahlung durchstrahlt hierbei die Einzeltropfensäule und trifft auf eine CCD-Zeilenkamera, die erlaubt es die Einzeltropfengröße sowie -geschwindigkeit messtechnisch zugänglich zu machen. Die Zeilenkamera wurde mit einer entsprechenden Optik ausgestattet um den relevanten Wellenlängenbereich zugänglich zu machen. Es lassen sich zeitliche Auflösungen im ms-Bereich realisieren.

CPP 2.6 Mon 11:00 H40

Grenzflächeneffekte: Gezielte Nutzung zur Herstellung von Nanopartikeln in Miniemulsionen — ●MARION WINKELMANN¹, REINHARD MILLER² und HEIKE P. SCHUCHMANN¹ — ¹Karlsruher Institut für Technologie, Lebensmittelverfahrenstechnik — ²Max-Planck-Institut für Kolloid- und Grenzflächenforschung

In dem vorgestellten Miniemulsionsverfahren wird zunächst eine W/O-Miniemulsion hergestellt und dabei ein wasserlöslicher Reaktand in der Dispersphase vorgelegt. Danach wird die Miniemulsion mit einem amphiphilen Reaktanden versetzt, der über die von Emulgator belegte Grenzfläche in die Miniemulsionstropfen diffundiert und damit die Partikelbildung durch eine Fällungsreaktion auslöst. Unsere Ergebnisse zeigen, dass die Anwesenheit von Emulgator an der Flüssig/Flüssig-Grenzfläche den Stoffübergang aus der öligen in die wässrige Phase beeinflusst. Entscheidend ist zusätzlich, ob die Grenzfläche belegt oder zunächst unbelegt von Emulgator ist. Liegt eine belegte Grenzfläche vor, wie für die Gewährleistung der Emulsionsstabilität erforderlich, so adsorbiert vergleichsweise weniger Reaktand an die Grenzfläche. Stehen hingegen Reaktand und Emulgator in direkter Konkurrenz um die unbelegte Grenzfläche, befindet sich anteilmäßig mehr Reaktand in der Grenzfläche. Die Grenzflächenbelegung wird somit nicht nur von den Adsorptions- und Desorptionseigenschaften des Reaktanden beeinflusst, sondern auch durch die Prozessführung. Die Prozessführung beeinflusst demnach maßgeblich die Partikelbildung durch Fällung in Miniemulsionen mit. Im Vortrag wird auch gezeigt, wie sich dies auf die resultierende Partikelgröße des gefällten Produkts auswirkt.

15 min. break

CPP 2.7 Mon 11:30 H40

Interfacial roughening and breakup of thin liquid films — ●MARKUS GROSS — ICAMS, Ruhr-Universität Bochum, Germany

A fluid interface in equilibrium is characterised by the presence of thermally excited capillary waves. However, in many cases, such as in phase-separation processes under shear or in pattern-forming systems, interfaces are initially not in equilibrium and it takes a certain time during which the interfaces roughens to reach its equilibrium state. Employing an effective Langevin formalism and simulations of the full fluctuating hydrodynamic equations, we first discuss the different dynamic universality classes of fluid interfacial roughening. Besides being a theoretically interesting non-equilibrium growth phenomenon, interfacial roughness has also important repercussions on the stability of thin films or liquid domains: if the surface tension is low, interfaces fluctuate violently and a breakup of the domain can result. So far, film breakup has typically been studied assuming the dominance of disjoining pressure. Here, we focus on the purely fluctuation-dominated regime, where the breakup is a "rare event" and effects of disjoining pressure are negligible at all times except close to the breakup.

CPP 2.8 Mon 11:45 H40

Between soap bubbles and vesicles: Dynamics of smectic bubbles — ●KATHRIN MAY, KIRSTEN HARTH, TORSTEN TRITTEL, and

RALF STANNARIUS — Institute of Experimental Physics, Faculty of Natural Sciences, Otto von Guericke University Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Smectic bubbles are ideal model systems to study thin closed liquid membranes. A preparation technique for these meniscus-free smectic bubbles is presented. The initially oblong-shaped bubbles perform shape transformations towards the equilibrium sphere shape with minimum surface. The monitoring of these processes is done by optical high-speed imaging. Their shape transformations, especially the changes of the surface area, are analyzed and their dynamic characteristics are compared to classical soap bubbles and vesicles. Small submillimeter bubbles can be studied under normal gravity laboratory conditions. Larger bubbles have been investigated during parabolic flights, which provide a 22 s microgravity phase.

CPP 2.9 Mon 12:00 H40

Structure formation at μ - structured liquid/gas interfaces — ●HANS-GEORG BRAUN, RENE HENSEL, and ANDRE ZAMITH-CARDOSO — Leibniz Institute of Polymer Research Dresden - Max Bergmann Center of Biomaterials, D-01069 Dresden, Germany

Application of microheterogeneous surfaces easily prepared by soft-lithographic patterning techniques has provided deep insights into interfacial processes such as wetting or dewetting, nucleation at patterned solid/liquid interfaces. Much less is known about the formation of microstructured liquid/gas interfaces and their influence on interfacial self-organization processes. This contribution focuses on

- the preparation, surface modification and interfacial stability of floating microstructured polymer membranes by PRINT
- the interfacial stabilization of aqueous liquids by encapsulation in microparticles in so called Liquid marbles and the pH triggered self-organization of peptides into ultrathin gel layers at the liquid/gas interface into these liquid marbles.
- Finally the interfacial formation of floating calciumcarbonate rafts at the liquid / air interface will be discussed.

- R. Hensel and H.-G. Braun, *Soft Matter* 2012,8, 5293
- H.-G. Braun, A. Zamith-Cardoso, *Colloids and Surfaces: B Biointerfaces*, 2012, 97, 43-50

CPP 2.10 Mon 12:15 H40

Imaging of carbon nanomembranes and graphene with helium-ion microscopy — ●ANDRÉ BEYER, HENNING VIEKER, ANNIKA WILLUNAT, NILS-EIKE WEBER, MATTHIAS BÜENFELD, ANDREAS WINTER, XIANGHUI ZHANG, MIN AI, ANDREY TURCHANIN, and ARMIN GÖLZHÄUSER — Physics of Supramolecular Systems, University of Bielefeld, 33615 Bielefeld, Germany

We present a helium-ion microscopy (HIM) study of carbon nanomembranes (CNMs) and graphene. CNMs are extremely thin (~1 nm) nanolayers consisting only of surface-near atoms. They are made via cross-linking of self-assembled monolayers (SAMs) with large-area exposures of electrons, photons or helium ions and subsequent transfer to suitable substrates. In this contribution we demonstrate that imaging of CNMs with HIM is an effective way of their characterization due to the high surface sensitivity of HIM. Patterned radiation exposures allow the fabrication of perforated nanomembranes, e.g. nanosieves. Another way of generating nanopores in homogeneous CNMs is to irradiate them with slow highly charged ions. Imaging such perforated CNMs with HIM yields high signal-to-noise ratios as well as low sample damage. Annealing of CNMs at high temperatures in vacuum transforms them into graphene. HIM images of graphene from SAMs are compared with CVD grown graphene. Capabilities of HIM imaging of freestanding CNMs and graphene will be discussed.

CPP 2.11 Mon 12:30 H40

Structure of nano-phase separated monomolecularly thick water-ethanol layers confined between graphene and mica — ●NIKOLAI SEVERIN, VITALIJ SCENEV, PHILIPP LANGE, IGOR M. SOKOLOV, and JÜRGEN P. RABE — Department of Physics, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

Understanding and control of liquids confined to the nano-scale is of wide interest, e.g., for molecular assays and synthesis to be performed on small scales. We report in-situ scanning force microscopy imaging of graphenes replicating nano-phase separated ethanol-water monomolecular films on an atomically flat mica surface. Graphenes conform to the film topography bending at the boundaries between domains of water and the larger ethanol molecules. The lateral size of molecular domains becomes larger with the graphene thickness, which we attribute to the

graphene bending energy. Ethanol and water molecules have been demonstrated to dope graphene negatively and positively, respectively [1]. Consequently, we account for stabilization of the heterogeneity by the counteraction of electrostatic repulsion of the doped charges and line tension controlled by the bending energy of the graphene layers. 1. Schedin, F., et al., *Nature Materials*, 6 (2007) 652.

CPP 2.12 Mon 12:45 H40

Gas permeation through PDMS membranes covered by 2D carbon nanomembranes (CNMs) — ●MIN AI¹, SERGEY SHISHATSKIY², JAN WIND², ANDRÉ BEYER¹, NILS MELLECH¹, ANDREAS WINTER¹, HENNING VIEKER¹, JUN QIU³, and ARMIN GÖLZHÄUSER¹ — ¹Physics of Supramolecular Systems of Surfaces, Bielefeld University — ²Institute of Polymer Research, Helmholtz-Zentrum Geesthacht — ³DSM, The Netherlands

Polymeric ultra-thin films are promising candidates to be used as components in miniaturized electronic, medical or energy devices. In this contribution, we report the fabrication of ultra-thin (~1 or 3 nm) carbon nanomembranes (CNMs). Organic self-assembled monolayers were irradiated by electrons, leading to a two-dimensional cross-linked CNM through dehydrogenation and recombination mechanisms [1]. The 1-nm- or 3-nm-thick CNMs with an area of 1.2 square centimeters were then transferred onto polydimethylsiloxane (PDMS) composite membranes. The CNM-PDMS membranes were analyzed by XPS, SFM and Helium Ion Microscopy. Gas permeances of H₂, He, CO₂, O₂, N₂, Ar, CH₄, C₂H₆ were measured using "constant volume variable pressure" technique. The new CNM-PDMS composite membranes exhibited significantly lower permeances for all the gases than the PDMS composite membrane and different gas selectivities from the PDMS membrane.

[1] A. Turchanin, D. Käfer, M. El-Desawy, Ch. Wöll, G. Witte, A. Gölzhäuser, *Langmuir* 25, 7342 (2009).

CPP 2.13 Mon 13:00 H40

Living polymer system in contact with a solid substrate. — ●DEWEN SUN and MARCUS MÜLLER — Institut für Theoretische Physik der Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077, Göttingen, Niedersachsen, Deutschland

Systems, in which polymerization takes place under the condition of chemical equilibrium between polymers and their respective monomers are termed "living polymer systems". The reversible bonding gives rise to a chain length polydispersity in these complex polymer fluids. Using computer simulation of a soft, coarse-grained model, we investigate how the presence of a solid substrate influences the behavior of living polymer system in the narrow interface between a solid substrate and a polymer melt and in the wider interphase region. We observe that the contact with a solid substrate in a film geometry alters the local mean molecular weight and the local molecular weight distribution and we discuss the changes as a function of the scission energy.

CPP 2.14 Mon 13:15 H40

Fast formation of roughness correlation in thin spray-coated polystyrene homopolymer film — ●JAN PERLICH, ADELIN BUFFET, MATTHIAS SCHWARTZKOPF, GERD HERZOG, BERIT HEIDMANN, STEPHAN V. ROTH, and RAINER GEHRKE — Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, D-22607 Hamburg (Germany)

Thin polymer films form smooth films with correlated interfaces, so-called conformal roughness, under suitable preparation conditions in dependence of the polymer characteristics [1,2]. The directed replication of the substrate features to a certain cut-off length is highly desirable. Hence, insight into the formation process is required. We present the fabrication of such a thin film of a polystyrene homopolymer via spray-coating. The spray-coating process is monitored in situ real-time by microbeam grazing incidence small angle X-ray scattering (microbeam-GISAXS) performed at the synchrotron beamline P03 (MiNaXS) of PETRA III (DESY) in Hamburg [3]. The dedicated in situ setup provides a time resolution in the millisecond regime enabling the observation of the fast formation of roughness correlation in the thin film upon drying of the polystyrene homopolymer solution. The recorded scattering signals reveal the information to extract the evolution of the correlation and cut-off lengths as well as the corresponding time constants in the formation process.

[1] P. Müller-Buschbaum et al., *Macromolecules* 31 (1998) 3686.

[2] J. S. Gutmann et al., *Physica B* 283 (2000) 40.

[3] A. Buffet et al., *J. Synchrotron Rad.* 19 (2012) 647.

CPP 3: Charge Transfer Effects in Molecular Materials I (joint session CPP/HL/BP/DS)

Related to SYCT organized by Frank Schreiber (Tübingen) and Wolfgang Brütting (Augsburg).

Time: Monday 12:15–13:30

Location: H1

CPP 3.1 Mon 12:15 H1

Thermally Activated Intermixing in Pentacene - Perfluoropentacene Heterostructures — ●TOBIAS BREUER and GREGOR WITTE — Molekulare Festkörperphysik, Philipps-Universität Marburg, Renthof 7, 35032 Marburg

We report on the thermal stability of pentacene (PEN, C₂₂H₁₄) and perfluoropentacene (PFP, C₂₂F₁₄) heterostructures. We show that the thermal stability of the heterostructure compared to the single compounds is significantly enhanced by about 20 K. By varying preparation methods and stoichiometric ratios of the heterostructures we show that the stabilization is restricted to heterostructures with stoichiometric ratio of 1:1. Moreover, the thermal stabilization strongly depends on the preparation method, especially the deposition sequence of both materials in subsequent stacks. While PFP as bottom and PEN as top layer yield stabilized layers, no such effect is found for PEN as bottom layer and PFP on top. This asymmetry of intermixing and corresponding morphological information obtained by means of AFM measurements as well as optical absorption spectra as benchmark for hetero-interaction are discussed. The results are compared to additional preparation methods of heterostructures like co-evaporation and post-deposition-annealing.

CPP 3.2 Mon 12:30 H1

Mixing-induced anisotropic correlations in molecular crystalline systems: Rationalizing the behavior of organic semiconductor blends — ●KATHARINA BROCH, ANTJE AUFDERHEIDE, JIŘÍ NOVÁK, ALEXANDER HINDERHOFER, RUPAK BANERJEE, ALEXANDER GERLACH, and FRANK SCHREIBER — Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

Binary mixtures of organic semiconductors (OSCs) have recently be-

come an important field of research, as they find applications in optoelectronic devices [1]. In these systems, the mixing (intermixing vs. phase separation) and ordering behavior is crucial, since it affects the optical and electronic properties including the degree of charge-transfer (CT). We present a comprehensive study of binary mixtures of the three prototypical OSCs pentacene (PEN), perfluoropentacene (PFP) and diindenoperlyene (DIP) in all possible combinations [1,2,3]. Using X-ray reflectivity and grazing incidence X-ray diffraction we investigate the structural properties of the mixed films as well as their impact on the optical spectra obtained by spectroscopic ellipsometry. For PEN:DIP we find an anisotropic ordering behavior, comparable to that observed in some liquid crystals, which is fundamentally new for OSCs [2]. The influence of sterical compatibility and the strength of the intermolecular interactions on the mixing and ordering behavior in the different blends will be discussed by extending a conventional mean-field model [1]. [1] A. Hinderhofer and F. Schreiber, *Chem.Phys.Chem.*, **13**, 628 (2012); [2] A. Aufderheide et al., *Phys.Rev.Lett.*, **109**, 156102 (2012); [3] J. Reinhardt et al., *J.Phys.Chem. C*, **116**, 10917 (2012)

CPP 3.3 Mon 12:45 H1

Screening Effects on Excitation Energy Transfer in Supramolecular Complexes in a Mixed Quantum Classical Description — ●JÖRG MEGOW¹, THOMAS RENGER², and VOLKHARD MAY¹ — ¹Humboldt-Universität zu Berlin, Deutschland — ²Johannes Kepler Universität Linz, Österreich

Excitation energy transfer (EET) within the supramolecular complex P16 (sixteen pheophorbide a molecules covalently linked to a DAB-dendrimer) is studied using a mixed quantum classical methodology [1,2] that takes the screening of excitonic coupling into account. The excitonic coupling between two chromophores is calculated as Coulomb-coupling between transition partial charges. This treatment neglects

the screening effects due to interaction with the solvent molecules. The Poisson-TrEsp (transition charges from electrostatic potentials) method [3], developed in the group of Renger, allows the calculation of screening factors that correct the excitonic coupling between two chromophores dependent on their distance, mutual orientation and conformation. A new method is proposed that allows to obtain the orientation and conformation dependence of the Poisson-TrEsp screening factors in a mixed quantum-classical description by introducing a novel fitting procedure. While all screening ansatzes result in a deceleration of the EET, the new approach results in a considerable acceleration of the EET compared to standard screening approaches.

[1] J. Megow et al., *ChemPhysChem* 12, 645 (2011) [2] J. Megow et al., *Chem. Phys.* 377, 10 (2010) [3] J. Adolphs et al., *Photosynth. Res.* 95 (2008)

CPP 3.4 Mon 13:00 H1

In operando STXM investigations of charge carriers in SAM-FET devices — ●ANDREAS SPÄTH¹, THOMAS SCHMALTZ², BENJAMIN WATTS³, MARCUS HALIK², and RAINER H. FINK¹ — ¹FAU Erlangen-Nürnberg, Physical Chemistry II, Erlangen, Germany — ²FAU Erlangen-Nürnberg, Polymer Sciences, Erlangen, Germany — ³Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland

Based on previous work on pentacene based organic FETs [1], we present first results of zone plate scanning transmission soft x-ray microspectroscopy (STXM) on novel organic devices based on self assembled monolayers (SAMs). STXM combines high lateral resolution and spectroscopic sensitivity. Electron detection is used to achieve surface sensitivity, thus offering access to monolayer films. The SAMs implement all functionalities of the FET, i.e. gate dielectric and organic semiconductor [2]. STXM analysis within the active channel during operation of the SAMFET shows small variations in the electronic structure which are interpreted in terms of field induced shifts

of the electronic levels and/or local charges. The unique combination of STXM and AFM provided by the NanoXAS beamline at the Swiss Light Source enables us to monitor both, the morphological homogeneity of the SAM film and modifications in the electronic structure. Thus, a more detailed insight into the correlation of morphological and electronic properties of these ultrathin devices can be achieved. The project is funded by the BMBF (contract 05K10WEA).

[1] C. Hub, et al., *J. Mater. Chem.* 20, 2010, 4884

[2] A. Rumpel, et al., *Langmuir* 27, 2011, 15016

CPP 3.5 Mon 13:15 H1

Scanning Kelvin Probe Microscopy on FIB-milled Cross Sections of Organic Solar Cells — ●REBECCA SAIVE^{1,2,3}, CHRISTIAN MÜLLER^{1,2,3}, MICHAEL SCHERER^{1,2,3}, DOMINIK DAUME^{1,2,3}, MICHAEL KRÖGER^{1,3}, and WOLFGANG KOWALSKY^{1,2,3} — ¹InnovationLab GmbH, Heidelberg, Germany — ²Kirchhoff-Institut für Physik, University Heidelberg, Germany — ³Institut für Hochfrequenztechnik, Technische Universität Braunschweig, Germany

Scanning Kelvin probe microscopy (SKPM) is a promising tool to analyze charge carrier transport paths in electronic devices. Conventional SKPM is limited to analysis of charge transport parallel to the device surface, e.g. within planar field-effect transistors, whereas the transport in vertical devices e.g. bulk heterojunction solar cells is not accessible to further characterization. Therefore we introduce a method to directly measure at the cross sections of organic devices by milling with a focused ion beam (FIB) and adjacent SKPM characterization. By this method we can reveal a spatially resolved potential distribution and therefore identify charge injection and charge transport barriers. In this work, we could correlate microscopic measurement results like the work function difference between the contact materials to macroscopic device characteristics received by J-V measurements and impedance spectroscopy.

CPP 4: SYBD: Magnetic Nanoparticles in Biomedical Diagnostics and Therapy

Time: Monday 15:00–17:30

Location: H1

Invited Talk

CPP 4.1 Mon 15:00 H1

Functionalization and Pharmaceutical Aspects of Magnetic Nanoparticles (Magnetic Carriers) — ●URS O. HÄFELI — University of British Columbia, Faculty of Pharmaceutical Sciences, Vancouver, BC, Canada

This presentation will review the properties and applications of modern magnetic nanoparticles and microspheres for application as nanomedical agents, both for diagnosis and therapy of different diseases. Basic applications in biomedicine and industry, clinical applications, as well as open questions regarding risk and economy will be discussed.

Important features make nanoparticles and microspheres interesting for in vitro and in vivo applications: biocompatibility, biodegradability, transport capacity, surface functionalization with biological active molecules, binding of fluorescent and radioactive markers, increasing surface area with decreasing size, organ-specific targeting.

To further increase the particles efficiency, further work is necessary in the design of effective magnetic targeting systems, the coatings for optimized particles, the choice of targeting ligands, as well as the maximization of the particles* magnetic moment. Altogether, exciting in vivo applications are possible in magnetic guidance and controlled delivery of drugs, genetic material, and stem cells, in addition to their current use for the contrast enhancement in magnet resonance imaging and local hyperthermia treatment of cancer.

For additional information about the scientific field of magnetic particles, please check out www.magneticmicrosphere.com.

Invited Talk

CPP 4.2 Mon 15:30 H1

Fluid mechanical aspects of therapeutic application of suspensions of magnetic nanoparticles — ●STEFAN ODENBACH — TU Dresden, Chair of Magnetofluidynamics, Measuring and Automation Technology, Dresden, Germany

One of the promising approaches for the use of magnetic nanoparticles in cancer therapy is a technique called magnetic drug targeting. Here a chemotherapeutic agent is attached to the surfactant of the magnetic particles and a water based suspension of these drug carrying particles is injected into a supplying artery of the tumour. Using appropriate magnetic fields magnetic forces can be generated targeting the parti-

cles towards the tumour. As a result chemotherapy without side effects is envisaged.

Within the talk some of these aspects resulting from fluid mechanics will be highlighted and discussed. On the one hand we'll have a look on model experiments studying the targeting process for the magnetic fluid and its dependence on magnetic field configuration. The respective experiments presented will be accompanied by numerical simulations which are intended to provide a tool for future clinical applications allowing an optimal field control on the basis of angiographic data.

The second part of the talk will focus on magnetic field effects concerning the viscosity of ferrofluids for biomedical applications as well as on changes of the flow behaviour of blood with suspended magnetic particles in a field and will thus highlight investigations on fundamental fluid properties being important for experiments as well as simulations.

Invited Talk

CPP 4.3 Mon 16:00 H1

Magnetic Particle Imaging: A new Medical Imaging Modality — ●THORSTEN BUZUG — Institute of Medical Engineering, University of Lübeck, Germany

Recently, magnetic particle imaging (MPI) has been introduced as a novel method for direct measurement of the spatial distribution of superparamagnetic iron oxide nanoparticles (SPIOs) that are used as tracer material. The SPIOs are subjected to a sinusoidally oscillating magnetic field and respond with a nonlinear change in magnetization. The acquired induction signal contains harmonics of the fundamental excitation frequency, which are subsequently used for determination of the spatial particle distribution and concentration. For spatial encoding a magnetic gradient field (the selection field) is superimposed onto the sinusoidal excitation field (the drive field) such that a field-free point (FFP) is established at a desired location within the field of view. Nanoparticles located near the FFP contribute to the signal generation, whereas particles that are far from the FFP are in saturation and cannot contribute. Image reconstruction from the measured induction signals can be seen as the solution for the corresponding inverse problem. In this talk, the state of the art in magnetic coil design for MPI is discussed. With a new symmetrical arrangement of coils, a field-free line can be produced that promises a significantly higher

sensitivity compared with the standard arrangement for an FFP. Additionally, an alternative single-sided coil assembly is presented for the use in hand-held applications.

Invited Talk CPP 4.4 Mon 16:30 H1
Superparamagnetic iron oxide nanoparticles for MR-visible mesh implants and novel drug targeting models — ●IOANA SLABU^{1,2}, ANJALI ROETH³, CHRISTIANE KUHL⁴, THOMAS SCHMITZ-RODE¹, and MARTIN BAUMANN¹ — ¹Applied Medical Engineering, Medical Faculty, Helmholtz Institute, RWTH Aachen University, Germany — ²II. Physical Institute, RWTH Aachen University, Germany — ³Department of Surgery, University Hospital, RWTH Aachen University, Germany — ⁴Department of Radiology, University Hospital, RWTH Aachen University, Germany

Two major medical applications of superparamagnetic iron oxide (SPIO) nanoparticles are presented, exploiting their physical and magnetic properties to combine diagnostic and therapeutic functionalities. First, the concept and realization of a (magnetic resonance) MR-visible mesh implant is described which facilitates an accurate determination of complications after mesh implantation by means of MR imaging. The visual investigation of the implant helps to reduce the exposure of the patient to redundant surgery interventions. Second, magnetic drug targeting approaches based on numerical simulations for cancer therapies are developed. A new concept of placing an array of permanent magnets and coils inside hollow organs of the body very close

to tumors is described. In this way, a stronger magnetic field and its higher gradient are achieved in the tumor. This allows a local accumulation of administrated SPIO nanoparticles with bounded drugs and enhances the efficiency of the therapy. First simulation results are already applied and validated in animal trials.

Invited Talk CPP 4.5 Mon 17:00 H1
Magnetic measurement techniques assisting biomedical applications of magnetic nanoparticles — ●LUTZ TRAHMS — Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, D-10587 Berlin, Germany

Due to their biocompatibility and their small size, magnetic nanoparticles (MNP) made of iron oxide can be guided to virtually every biological environment. MNP are susceptible to external magnetic fields and can be used, e.g., for drug transportation, heat generation or as contrast agents for MRI. All these applications require knowledge about the magnetic properties and, when applied in-vivo, quantitative knowledge about the spatial distribution in the living tissue. In this contribution, I will report on a number of magnetic measurement techniques that provide such information, i.e. in particular on conventional susceptibility measurements $M(H)$, magnetorelaxometry, and magnetic particle spectroscopy. In addition, I will give examples how these analytical or spectroscopic techniques can be modified to obtain quantitative spatial information.

CPP 5: Glasses and Glass Transition I (joint session DY/CPP)

Time: Monday 15:00–17:30

Location: H34

Invited Talk CPP 5.1 Mon 15:00 H34
Intra- and inter-molecular dynamics in glass-forming liquids — ●PERIKLIS PAPAPOULOS¹, WILHELM KOSSACK², and FRIEDRICH KREMER² — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²Universität Leipzig, Germany

The intra- and inter-molecular interactions of salol and polystyrene, as low molecular weight and polymeric glass-forming model systems, are studied by Fourier-transform infrared (FTIR) spectroscopy and Broadband Dielectric Spectroscopy (BDS). By analysing the temperature dependencies of specific IR absorption bands it is demonstrated that each molecular moiety in the glass-formers has its own signature in the course of the dynamic glass transition: while some do not show any change at the calorimetric glass transition temperature, others exhibit a pronounced “kink”. The effects cannot be attributed solely to microscopic thermal expansion, but instead indicate gradual conformational changes. The ease of application of this approach to a variety of systems in different geometries and external conditions can assist the modelling of glasses and the understanding of the coupling between the glass transition and molecular-level dynamics.

[1] P. Papadopoulos, W. Kossack, and F. Kremer, *Soft Matter*, 2013, 9, 1600 - 1603

CPP 5.2 Mon 15:30 H34
In-situ investigation of vapor-deposited thin films of toluene and ethylbenzene by AC chip-nanocalorimetry — ●MATHIAS AHRENBERG¹, KATIE R. WHITAKER², YEONG-ZEN CHUA¹, HEIKO HUTH¹, MARK D. EDIGER², and CHRISTOPH SCHICK¹ — ¹Institut für Physik, Universität Rostock, Wismarsche Str. 43-45, 18051 Rostock, Germany — ²Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA

Physical vapor deposition can be used to produce thin films with particular material properties. For example extraordinarily stable glasses can be obtained from organic molecules like toluene and ethylbenzene. We have investigated properties like packing efficiency and kinetic stability depending on substrate temperature and deposition rate by in-situ AC chip-nanocalorimetry. We have varied the substrate temperature covering the range from temperatures proven to yield high enthalpy glasses up to temperatures proven to yield low enthalpy glasses. This way the complete evolution of the mentioned stable glass properties is observed. Moreover AC calorimetry offers the possibility for isothermal measurements which enables to follow the transformation of the stable glass to the super-cooled liquid. Transformation experiments give suggestion of the transformation mechanism and its temperature dependence. The data are in agreement with a growth front for the

transformation of the stable glass into the supercooled liquid.

CPP 5.3 Mon 15:45 H34
Calorimetric glass transition of ultrathin films of homopolymers and their blends — ●HUAJIE YIN and ANDREAS SCHÖNHALS — BAM Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12205 Berlin, Germany

Glass transition behavior of different ultrathin polymer films (down to around 10 nm) was investigated by specific heat spectroscopy using differential AC calorimetry. For thin homopolymer films like polystyrene (PS) and poly(vinyl methyl ether) (PVME), no thickness dependence of dynamic glass transition temperature was observed down to 10 nm. Furthermore, the width of the glass transition is independent of the film thickness which indicates that the extent of the cooperativity is essentially smaller than 10 nm. For polymer blend thin films in the case of PS/PVME with the weight fraction of 50/50, the dynamic glass transition temperature was found to be decreasing with reducing the film thickness. This phenomenon is explained in terms of surface enrichment of PVME in the polymer blend system where PVME has a lower surface energy than PS. X-ray photoelectron spectroscopy (XPS) was used to probe the surface composition in order to confirm such surface enrichment phenomena.

CPP 5.4 Mon 16:00 H34
Molecular dynamics of a discotic liquid crystal studied by Dielectric Relaxation and Specific Heat Spectroscopy — ●CHRISTINA KRAUSE¹, HUAJIE YIN¹, ANDREAS WURM², CHRISTOPH SCHICK², and ANDREAS SCHÖNHALS¹ — ¹BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, D-12205 Berlin — ²Institute of Physics, University of Rostock, Wismarsche Straße 43-45, D-18051 Rostock

The molecular dynamics of the discotic liquid crystal pyrene-1,3,6,8-tetracarboxylic tetra(2-ethylhexyl)ester is investigated by dielectric relaxation and specific heat spectroscopy. The data from dielectric spectroscopy shows 3 processes: a β -relaxation at low temperatures and an α -relaxation in the temperature range of the mesophases followed by conductivity. In both phases the dielectric α -relaxation is assigned to restricted glassy dynamics. Glassy dynamics is also detected in the plastic crystalline phase by means of specific heat spectroscopy but with a different temperature dependence of the relaxation rates. This is discussed considering the different molecular restrictions of the fluctuations: close to the columns (dielectric spectroscopy) and more in the intercolumnar space (specific heat spectroscopy). In the frame of the fluctuation approach a correlation length of glassy dynamics is calculated to 0.78 nm which correlates well to the core-core distance

estimated by X-ray scattering.

CPP 5.5 Mon 16:15 H34

Liquid to glass transition in a Wigner glass — ●FABIAN WEST-ERMEIER, MICHAEL SPRUNG, and GERHARD GRÜBEL — HASYLAB, Deutsches Elektronen-Synchrotron, 22607 Hamburg, Germany

One of the interesting problems of disordered systems is the nature of the liquid to glass transition. While the glass transition in molecular glass formers can be typically achieved by cooling down the system, in colloidal systems the glassy state is experimentally accessible by changing the strength of the direct particle interactions.

Colloidal systems can be distinguished by their type of interaction. While so called hard sphere systems interact via a repulsive, short range interaction potential, electrostatically stabilized systems are interacting via a long-range, screened Coulomb potential which depends inter alia on the charge of the particles and the concentration of additional ions in the solvent screening the direct particle interactions. As it is thus possible to tune the direct particle interaction strength of these systems, the glass transition can already occur at much lower volume fractions when compared to the hard sphere case.

We have used X-ray scattering techniques to investigate the glass transition of a charge stabilized system at a constant volume fraction, varying only the strength of the direct particle interactions. While the average structure of the colloidal suspensions shows only minor changes, the dynamics of the system vary strongly as a function of the direct particle interaction strength.

CPP 5.6 Mon 16:30 H34

Temporal evolution of structural and dynamical heterogeneities in a metastable colloidal fluid — ●SEBASTIAN GOLDE^{1,2}, MARKUS FRANKE², and HANS JOACHIM SCHÖPE^{2,3} — ¹Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany — ²Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Germany — ³MPI für Polymerforschung, Postfach 3148, 55021 Mainz, Germany

An interesting property of the metastable melt is that it exhibits spatial heterogeneous dynamics [1]. The dynamics can be understood as an accumulation of mobile and immobile particles. Recent work suggested that the local structure and dynamics of the metastable melt are correlated to each other [2]. In order to investigate these phenomena we used a hard sphere like colloidal model system. The local dynamics in the metastable colloidal melt were measured with our recently new designed multispeckle correlation spectroscopy setup which performs space- as well as time-resolved dynamic light scattering. The solidification kinetics was measured using an advanced time-resolved laser light Bragg scattering setup. The correlation between the particle dynamics and the solidification kinetics could be quantified by analyzing the temporal evolution of the local particle dynamics, the ensemble averaged dynamic structure factor and the solidification kinetics. Crossing the glass transition point we can show that there is fundamental link between crystallization and vitrification. [1] L. Berthier and G. Biroli, *Rev. Modern Physics* 83 (2011), [2] T. Kawasaki and H. Tanaka, *JCPM* 22 (2010)

CPP 5.7 Mon 16:45 H34

Multiple reentrant glass transitions in confined hard-sphere glasses — ●SUVENDU MANDAL^{1,2}, SIMON LANG³, ROLF SCHILLING⁴, VITALIE BOTAN⁴, MARTIN OETTEL⁴, DIERK RAABE¹, THOMAS FRANOSCH³, and FATHOLLAH VARNIK^{1,2} — ¹Max-Planck Institut für Eisenforschung, Max-Planck Str. 1, 40237 Dusseldorf, Ger-

many — ²Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Stiepel Strasse 129, 44801 Bochum, Germany — ³Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058, Erlangen, Germany — ⁴Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany

We perform molecular dynamics simulations for a polydisperse, densely packed hard-sphere fluid confined between two parallel walls [1]. The diffusion coefficient parallel to the walls is observed to vary by orders of magnitudes upon changing the wall separation while keeping the packing fraction fixed. A striking multiple reentrance scenario emerges for the transition from liquid to glass as the wall separation becomes comparable to the particle diameter. The non-monotonic behavior of the phase diagram is rationalized in terms of a numerical solution of a recently developed mode-coupling theory [1,2].

[1] S. Mandal, S. Lang, R. Schilling, V. Botan, M. Oettel, D. Raabe, T. Franosch, and F. Varnik submitted [2] S. Lang, V. Botan, M. Oettel, D. Hajnal, T. Franosch, R. Schilling *PRL* 105, 125701 (2010).

CPP 5.8 Mon 17:00 H34

Shear banding in hard sphere glasses — SEGUN AYODELE¹, DIERK RAABE¹, INGO STEINBACH², and ●FATHOLLAH VARNIK^{1,2} — ¹Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — ²ICAMS, Ruhr Universität Bochum, Germany

When an amorphous solid is exposed to a simple shear such as a planar Couette flow, the flow may become heterogeneous despite the fact that the macroscopic stress is constant across the system [1,2]. However, both in computer simulations [1,3] and experiments [2] the observed velocity profile is unsteady with significant spatio-temporal fluctuations. In this work, we address the question whether a steady shear banded solution may exist. For this purpose, we both perform an analysis of the underlying equations as well as lattice Boltzmann simulations, using as input the constitutive laws obtained from MD simulations [3].

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

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

[3] S. Mandal, M. Gross, D. Raabe, F. Varnik, *Phys. Rev. Lett.* 108, 098301 (2012).

CPP 5.9 Mon 17:15 H34

Re-establishment of the equipartition theorem for small systems in molecular dynamics ensemble — ●NIMA HAMIDI SIBONI^{1,2}, DIERK RAABE², and FATHOLLAH VARNIK³ — ¹AICES, RWTH-Aachen, Germany — ²Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — ³ICAMS, Ruhr-Universität Bochum, Germany.

It has been reported recently that, in molecular dynamics (MD) simulations, periodic boundary condition leads to a violation of the equipartition theorem for systems containing particles with different masses [Shirts et al, *J. Chem. Phys.* **125** 164102 (2006)]. This effect is associated with the finite number of particles in MD simulations. Here, we propose a modification to MD simulation, which removes this problem. Our method is based on imposing Gaussian random fluctuations on the system's center of mass velocity. Using the analogy to a system exchanging momenta with impenetrable walls, we work out an analytical expression for the rate at which fluctuations are added to the system. The restoration of the equipartition is then demonstrated for small systems both at equilibrium as well as beyond equilibrium in the linear response regime.

CPP 6: Charge Transfer Effects in Molecular Materials II (joint session CPP/HL/BP/DS)

Related to SYCT organized by Frank Schreiber (Tübingen) and Wolfgang Brütting (Augsburg).

Time: Monday 15:00–17:30

Location: H40

Invited Talk

CPP 6.1 Mon 15:00 H40

a molecular picture of charge-transfer processes at donor-acceptor interfaces in organic solar cells — ●JEAN-LUC BREDAS — School of Chemistry and Biochemistry/Center for Organic Photonics and Electronics, Georgia Institute of Technology, Atlanta, Georgia 30332-0400

Our objective in this presentation is two-fold. First, after a general

introduction to organic solar cells, we use a molecular mechanics / molecular dynamics simulations approach to try and provide a molecular picture of the packing configurations (local morphology) at the interface between the donor and acceptor components in organic solar cells [1-3]. Then, we discuss in detail the impact that these local packing configurations at the interfaces have on the exciton-dissociation and charge-separation processes [4]. Systems under consideration include

fullerene derivatives or n-type oligoacene derivatives as acceptors and low optical-gap polymers or small molecules (pentacene or squaraine derivatives) as donors.

References (1) N. Cates Miller, E. Cho, et al., *Advanced Materials*, in press (DOI: 10.1002/adma.201202293). (2) N. Cates Miller, E. Cho, et al., *Advanced Energy Materials*, in press (DOI: 10.1002/aenm.201200392). (3) Y.T. Fu, C. Risko, and J.L. Bredas, *Advanced Materials*, in press (DOI: 10.1002/adma.201203412). (4) J.L. Bredas, J. Norton, J. Cornil, and V. Coropceanu, *Accounts of Chemical Research* 42, 1691 (2009).

CPP 6.2 Mon 15:30 H40

Microscopic simulations of charge transport in disordered organic semiconductors — ●DENIS ANDRIENKO, BJOERN BAUMEIER, PASCAL KORDT, ANTON MELNYK, and CARL POELKING — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Charge carrier dynamics in an organic semiconductor can often be described in terms of charge hopping between localized states. The hopping rates depend on electronic coupling elements, reorganization energies, and driving forces, which vary as a function of position and orientation of the molecules. The exact evaluation of these contributions in a molecular assembly is computationally prohibitive. Various, often semi-empirical, approximations are employed instead. Here, we review the current status of methods used to evaluate energetic disorder in organic semiconductors, such as polarizable force-fields and QM/MM approaches, focusing on their predictive power and accuracy. All methods are illustrated on donor-acceptor small-molecule interfaces as well as crystalline mesophases of conjugated polymers.

CPP 6.3 Mon 15:45 H40

Metal-Molecule Charge Transfer through Surface-Induced Conjugation — ●GEORG HEIMEL¹, STEFFEN DUHM², INGO SALZMANN¹, ALEXANDER GERLACH³, ANTJE VOLLMER⁴, FRANK SCHREIBER³, and NORBERT KOCH¹ — ¹Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — ²Institute of Functional Nano & Soft Materials, Soochow University, Suzhou 215123, P. R. China — ³Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — ⁴Helmholtz Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany

For the majority of large π -conjugated molecules, the Fermi level of supporting coinage-metal substrates is *pinned* to stay well within their electronic energy gap. In some cases, however, the Fermi level *does* cross into either of the frontier molecular orbitals. On the basis of a combined multi-technique experimental and theoretical study on a particularly clear-cut case – pentacenequinone and pentacenetetrone on the (111) surfaces of Au, Ag, and Cu – we present an attempt for a unifying explanation of such intriguing cases: The conjugation length of the organic semiconductor increases through interaction of specific chemical substituents with the metal surfaces. The ensuing reduction of the energy gap is found to be *the* crucial ingredient needed to overcome Fermi-level pinning. Our findings aid in the design of charged molecular monolayers, which are of interest both from the fundamental- and the applied-physics point of view.

Invited Talk CPP 6.4 Mon 16:00 H40
High efficiency OLEDs based on delayed fluorescence — ●CHIHAYA ADACHI — OPERA, Kyushu University, Fukuoka, Japan

We achieved a novel pathway to reach the ultimate EL efficiency by inventing simple aromatic compounds displaying efficient thermally-activated delayed fluorescence (TADF) with high photoluminescence efficiency, namely *hyperfluorescence*. While we had previously assumed that the S1 level should be significantly higher than the T1 level, i.e., 0.5–1.0 eV higher, due to the presence of electron exchange energy, we found that the proper design of organic molecules can lead to a small energy gap (Δ EST) between them. Relatedly, a molecule displaying efficient TADF requires a very small Δ EST between its S1 and T1 excited states, resulting in enhanced T1 * S1 reverse intersystem crossing (ISC). Such excited states are attainable by the intramolecular charge transfer (CT) of a spatially separated donor and acceptor system. The critical point of the molecular design is the compatibility of a small Δ EST \sim 0 eV and a reasonable radiative decay rate of over 10⁶/s that overcomes competitive non-radiative decay paths, leading to highly luminescent TADF materials. Since the two properties conflict with each other, a delicate balance of the overlap of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular

orbital (LUMO) is required. Furthermore, to enhance the PL efficiency of a TADF material, geometrical change between its S0 and S1 states should be restrained to suppress non-radiative decay processes. In this work, we designed a novel series of highly efficient TADF emitters that resulted in very high electroluminescence efficiency.

CPP 6.5 Mon 16:30 H40

Triplet Exciton Generation and Electron Back Transfer in Organic Solar Cells — ●ANDREAS SPERLICH¹, HANNES KRAUS¹, STEFAN VÄTH¹, ALEXANDER FÖRTIG¹, CARSTEN DEIBEL¹, and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²ZAE Bayern, 97074 Würzburg

To increase the power conversion efficiency of organic solar cells it would be extremely advantageous to improve the harvesting of singlet and charge transfer (CT) excitons. Dissociation of CT complexes into free charge carriers or, alternatively, their decay by electron back transfer (EBT) reactions depend on the energy levels of constituting donor and acceptor molecules, on microscopic structure of blends but also on the relative spin orientation of charges carriers within the e-h pair. We report on state-of-the-art organic semiconductors for polymer-fullerene bulk hetero-junction solar cells, such as blends based on the benzodithiophene donor PTB7 or the endohedral fullerene-derivative Lu₃N@C₈₀-PCBEH. We applied optical, current-voltage, morphology, and spin-sensitive techniques and found correlations between electrical performance of solar cells and formation of CT and triplet states. Combining results of these complementary experiments, we offer a physical picture on how pushing up the LUMO level of acceptors or tailoring the blends' morphology may end up in unwanted loss mechanisms in bulk-heterojunction solar cells.

CPP 6.6 Mon 16:45 H40

Reduced recombination and field independent charge carrier generation in polymer-polymer solar cells — ●STEFFEN ROLAND¹, MARCEL SCHUBERT¹, ZHIHUA CHEN², ANTONIO FACCHETTI², and DIETER NEHER¹ — ¹University of Potsdam, Institute of Physics and Astronomy — ²Polyera Corporation

Charge transport and recombination are investigated for solar cells made of poly(3-hexylthiophene) (P3HT) and the non-fullerene, high mobility acceptor copolymer P(NDI2OD-T2). Optimized devices show high fill factors of up to 70%, indicating that the excellent electron transport properties of pure P(NDI2OD-T2) is prevailed in the blend. By applying of the time delayed collection field technique (TDCF) we measured the field dependence of the charge carrier generation, and of the non geminate recombination as well as the electron and hole mobilities. The results reveal a field-independent photocurrent generation and a strongly reduced recombination coefficient for free charge carriers. The results imply that major charge carrier losses originate from an ultrafast (geminate) recombination on time scales below 10 ns.

Invited Talk CPP 6.7 Mon 17:00 H40

The role of intermolecular hybridization in molecular electrical doping — ●INGO SALZMANN¹, GEORG HEIMEL¹, HENRY MÉNDEZ¹, ANDREAS OPITZ¹, PATRICK BARKOWSKI¹, MARTIN OEHZELT^{2,1}, KATREIN SAUER¹, and NORBERT KOCH^{1,2} — ¹Humboldt Universität zu Berlin — ²Helmholtz Zentrum Berlin, Germany

Molecular electrical doping of functional organic semiconductor (OSC) films is typically done by the admixture of strong molecular donors/acceptors as dopants. In a recent combined experimental and theoretical study on prototypical OSC/dopant pairs we showed that positive polarons, evidencing the common perception of direct electron transfer between the highest occupied molecular orbital (HOMO) of the OSC and the lowest unoccupied molecular orbital (LUMO) of the p-dopant, are not observed in ultraviolet photoelectron spectroscopy even at considerable dopant ratios [1]. Instead of mutual ionization leading to singly occupied states, frontier molecular orbital hybridization between the OSC-HOMO and the dopant-LUMO occurs forming a *doubly occupied* bonding and an *empty* anti-bonding supramolecular hybrid orbital with a reduced fundamental gap, which is tunable by the acceptor strength. As all available states are occupied following Fermi-Dirac statistics, only a fraction of the hybrids is ionized at room temperature rationalizing the high dopant concentrations in practical applications. From this model, controlling the degree of hybridization emerges as strategy for the design of future improved molecular dopants in organic electronic devices.

[1] I. Salzmänn, G. Heimel et al., *Phys. Rev. Lett.* 108, 035502, 2012.

CPP 7: Organic Electronics and Photovoltaics I (joint session DS/CPP/HL/O)

Time: Monday 17:15–18:45

Location: H32

CPP 7.1 Mon 17:15 H32

Correlation between interface energetics and open circuit voltage in organic photovoltaic cells — ●ANDREAS WILKE¹, JAMES ENDRES², ULRICH HÖRMANN³, JENS NIEDERHAUSEN¹, RAPHAEL SCHLESINGER¹, JOHANNES FRISCH¹, PATRICK AMSALEM¹, JULIA WAGNER³, MARK GRUBER³, ANDREAS OPITZ¹, ANTJE VOLLMER⁴, WOLFGANG BRÜTTING³, ANTOINE KAHN², and NORBERT KOCH^{1,4} — ¹Humboldt-Universität zu Berlin, Institut für Physik, Brook-Taylor-Str. 15, D-12489 Berlin, Germany — ²Department of Electrical Engineering, Princeton University, Princeton, NJ 08544, USA — ³Universität Augsburg, Institut für Physik, Universitätsstr. 1, D-86135 Berlin, Germany — ⁴Helmholtz-Zentrum Berlin für Materialien und Energie GmbH BESSY II, Albert-Einstein-Str. 15, D-12489 Berlin, Germany

We have used ultraviolet and inverse photoemission spectroscopy to determine the transport gaps (E_T) of C60 and diindenoperylene (DIP), and the photovoltaic gap (E_{PVG}) of five prototypical donor/acceptor interfaces used in organic photovoltaic cells (OPVCs). The transport gap of C60 (2.5 ± 0.1) eV and DIP (2.55 ± 0.1) eV at the interface is the same as in pristine films. We find nearly the same energy loss of ca. 0.5 eV for all material pairs when comparing the open circuit voltage measured for corresponding OPVCs and E_{PVG} .

CPP 7.2 Mon 17:30 H32

Direct Observation of Charge Separation in Perylene Monoimide Solid State Dye-Sensitized Solar Cells — ●IAN HOWARD¹, MICHAEL MEISTER¹, BJÖRN BAUMEIER¹, HENRIKE WONNENBERGER¹, NEIL PSCHIRER², RÜDIGER SENS², INGMAR BRÜDER², KLAUS MÜLLEN¹, DENIS ANDRIENKO¹, and FRÉDÉRIC LAQUAI¹ — ¹Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany — ²BASF SE

Combining Vis-NIR broadband pump-probe transient absorption spectroscopy with precise measurement of the time-resolved photoinduced Stark effect we demonstrate that it is possible to track not only the rate of charge injection but also the motion of carriers after injection on the critical nanosecond timescale in Solid State Dye Sensitized Solar Cells. In terms of solar cell efficiency our findings have two major impacts. Firstly, we directly observe that the *reductive quenching* pathway previously suggested (wherein a photoexcited dye donates a hole to the hole transport material before then injecting an electron, now from the dye anion state, into the TiO₂) is important for obtaining high device efficiencies, especially for NIR absorbing dyes which exhibit a reduced driving force for electron injection directly from the dye exciton. Secondly, we find that many charges return to the interface after following injection, likely due to Coulombic and image charge effects. Screening the charges better, for example by reducing the dielectric contrast or increasing the dye length, should decrease the interfacial charge density and thereby parasitic recombination.

CPP 7.3 Mon 17:45 H32

Full electronic structure across a polymer heterojunction solar cell: interface dipoles and influence of light — ●JOHANNES FRISCH¹, PATRICK AMSALEM¹, JENS NIEDERHAUSEN¹, MARCEL SCHUBERT², EDUARD PREIS³, ANTJE VOLLMER⁴, JÜRGEN P. RABE¹, ULLRICH SCHERF³, DIETER NEHER², and NORBERT KOCH¹ — ¹Humboldt-Universität zu Berlin, Germany — ²Universität Potsdam, Germany — ³Bergische Universität Wuppertal, Germany — ⁴Helmholtz-Zentrum Berlin für Materialien und Energie - Speicherung BESSY II, Berlin, Germany

Controversial discussions concern the dependence of open circuit voltage on the energy offset between the highest occupied molecular orbital level of the donor material and the lowest unoccupied molecular orbital level of the acceptor material in organic photovoltaic cells. Therefore, we investigate the energy level alignment in two bilayer OPVCs comprising the donor poly(3-hexylthiophene) (P3HT) and the acceptors 1-(3-methoxycarbonyl)propyl-1-phenyl[6,6]C61 (PCBM) and poly(9,9'-dialkylfluorene-alt-4,7-bis(2,5-thiendyl))-2,1,3-benzothiadiazole (PFTBTT). Ultraviolet photoelectron spectroscopy revealed that notable interface dipoles occur at all interfaces across the OPVC structures for both material combinations. Particularly, the effective electrode work function (after contact formation with the organic material) differs significantly from those of the pristine mate-

rials. In addition, we find that negative charges are collected at the metal clusters (that exist in the early stage of cathode formation) due to exciton dissociation at the heterojunction.

CPP 7.4 Mon 18:00 H32

Optoelectronic Properties Of Zinc(II)-Phthalocyanine — ●MICHAEL KOZLIK, SÖREN PAULKE, MARCO GRUENEWALD, ROMAN FORKER, and TORSTEN FRITZ — University of Jena, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany

Zinc phthalocyanine (ZnPc) is an organic molecule which is used in organic optoelectronic devices, such as OLEDs and organic solar cells. Bulk material is represented mainly in form of the metastable α -ZnPc, while the stable β -ZnPc is less conductive [1]. We show the critical transformation temperature as well as optical and morphological differences between both phases. Description and simulation of the performance of organic devices make use of material parameters. In our work we present the determination of the optical constants and the exciton diffusion length. Experimental methods are UV-Vis spectroscopy and external quantum efficiency. By transmittance and reflectance spectra we derive the real and imaginary part of the refractive index [2]. In combination with the derived parameters we show the performance of a simplified photovoltaic cell and identify the region of exciton dissociation and exciton diffusion length.

References

- [1] K. Wilksne et al., J. Chem. Phys. 34 (1961) 2184.
- [2] M. Kozlik et al., Org. Electron. 13 (2012) 3291.

CPP 7.5 Mon 18:15 H32

The operational mechanism of ionic transition metal complex-based light-emitting electrochemical cells —

●SEBASTIAN B. MEIER^{1,2}, STEPHAN VAN REENEN³, HENK J. BOLINK⁴, MARTIJN KEMERINK³, WIEBKE SARFERT², and ALBRECHT WINNACKER¹ — ¹Department of Materials Science VI: Materials for Electronics and Energy Technology, University of Erlangen-Nuremberg, Germany — ²Siemens AG, Corporate Technology, CT RTC MAT MPV-DE, Erlangen, Germany — ³Department of Applied Physics, Eindhoven University of Technology, The Netherlands — ⁴Instituto de Ciencia Molecular, Universidad de Valencia, Spain

Light-emitting electrochemical cells (LECs) are promising candidates for cost-efficient next generation solid-state lighting and signage applications. They feature only a single, solution-processible active layer comprising a luminescent material in an ionic environment which allows for charge carrier injection from air-stable electrodes and low operating voltages. The operational mechanism of LECs has been the subject of an intense debate ever since their discovery. Evidence for electrochemical doping has been demonstrated for polymer-based devices, whereas LECs comprising ionic transition metal complexes (iTMCs) have almost exclusively been stated to operate via an electrodynamic mechanism. We used fluorescence as well as scanning Kelvin probe microscopy on planar iTMC-LECs to elucidate their mechanism of work. Our results illustrate profound evidence for electrochemical doping in these kind of LEC devices and highlight that the position of the established p-i-n junction is not fixed but migrates during device operation.

CPP 7.6 Mon 18:30 H32

Effective Charge Carrier Lifetimes in Organic Solar Cells Prepared by Coevaporation of C60 and CuPc in different mixtures and geometries — ●ANDRÉ DRAGÄSSER and DERCK SCHLETTWEIN — Institute of Applied Physics, Justus-Liebig-University Giessen, Giessen, Germany

Evaporated organic solar cells can lead to efficiencies of technical relevance if the interface of donor and acceptor molecules is optimized for the interplay of exciton dissociation, charge transport and recombination. The effective lifetime of the charge separated state is of central relevance. Intensity-modulated photovoltage spectroscopy with parallel impedance spectroscopy is a suitable method of analysis. Organic solar cells consisting of the well-established semiconductor materials CuPc and C60 were prepared by physical vapor deposition on an ITO substrate, modified with PEDOT:PSS. The cells were completed by a back contact of BCP as a buffer and aluminum. Cell architectures of planar junctions, bulk heterojunctions or planar-mixed hetero-

junctions were studied for different film thickness of the components. IV-measurements in the dark and under varied illumination intensities provided basic device characteristics. Detailed measurements of the short-circuit photocurrent and the open-circuit photovoltage under static or intensity-modulated illumination with different wavelength

were performed to determine the average charge carrier lifetime in the devices which was related to the respective charge carrier density obtained by impedance spectroscopy. Recombination reactions and, in particular, the influence of trap states will be discussed.

CPP 8: Poster: New Instruments and Methods

Time: Monday 17:30–19:30

Location: Poster C

CPP 8.1 Mon 17:30 Poster C

P62: A new small angle X-ray scattering instrument for the PETRA III Extension — ●JAN PERLICH, JAN RUBECK, RAINER GEHRKE, and SERGIO FUNARI — Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, D-22607 Hamburg (Germany)

Presently PETRA III is the most brilliant storage-ring-based X-ray radiation source in the world and thereby offers outstanding conditions for experiments with X-rays featuring small beam cross sections, high degree of collimation, and a wide range of photon energies. In the next years, the experimental facilities at PETRA III will be extended to provide additional instruments for various applications. This PETRA III Extension project will accommodate the new small angle X-ray scattering (SAXS) beamline P62 which is intended to comprise the large variety of X-ray scattering methods ranging from wide angle X-ray scattering (WAXS) to high-resolution ultra-small angle X-ray scattering (USAXS) in transmission and reflection geometry. Furthermore, the new instrument shall allow exploitation of anomalous X-ray scattering (ASAXS) with all setups and provide the option for simultaneous measurement in different angular scattering regimes. Due to the high photon flux available, time-resolved experiments down to milliseconds temporal resolution will be possible. We will present the characteristics and design parameters of the instrument and give a comprehensive overview of the experimental possibilities opened with this new instrument.

CPP 8.2 Mon 17:30 Poster C

Fluorescence Lifetime Imaging Microscopy in the Frequency Domain — ●STEPHANIE ZAHNER¹, LOTHAR KADOR¹, INGA ELVERS¹, JÜRGEN KÖHLER¹, KERIM R. ALLAHVERDI², and ELДАР YU. SALAEV³ — ¹University of Bayreuth, Institute of Physics and Bayreuther Institut für Makromolekülforschung (BIMF), Bayreuth, Germany — ²Marmara Research Centre of TÜBITAK, Materials Institute, Gebze/Kocaeli, Turkey — ³Azerbaijan National Academy of Sciences, Institute of Physics, Baku, Azerbaijan

A custom-built, low-cost Fluorescence Lifetime Imaging Microscope (FLIM) working in the frequency domain has been optimized and tested with three different materials. In addition to two-dimensional FLIM images, the results are shown in polar plot representation. Polymer matrices (PMMA and PVA) doped with Rhodamine 6G were used for characterizing the setup and the evaluation method. Films of the organic polymeric semiconductor P3HT show a distribution of short lifetimes below one nanosecond in combination with a longer lifetime component. The data points of the layered chalcogenide semiconductor Gallium-Selenid (GaSe) are spread over a wide range in the polar plot, some of them lying distinctly outside the semicircle. This effect is ascribed to the superlinear variation of the material's photoluminescence with the excitation light and has not been described in literature before.

CPP 8.3 Mon 17:30 Poster C

Characterization of heavy ion induced defects in ionic crystals by magnetic resonance techniques — ●MICHAEL DITTER, KAI-CHRISTIAN MEYER, SEBASTIAN ORTH, and FRANZ FUJARA — Institut für Festkörperphysik, TU Darmstadt, 64289 Darmstadt

We explore the potential and limitations of nuclear magnetic resonance (NMR) as a tool for the examination of heavy ion induced radiation damage in materials. We choose various fluoride crystals as guinea pig systems, here focusing at lithium fluoride (LiF). LiF offers two suitable probe nuclei for NMR, further on paramagnetic defects, such as F-centers, and metallic colloids can be observed directly by electron spin resonance (ESR). Extensive research has been carried out in the past but has also lead to new unanswered questions. NMR relaxometry with one dimensional spatial resolution is used to study defect generation and annealing behavior as well as impurity cluster

formation along and beyond the ion path. Data from conventional and spatially resolved NMR field-cycling experiments, the latter with a purposely built spectrometer [1], can be utilized to determine defect distribution. NMR spectroscopy is used to observe fluorine gas bubbles formed during irradiation. Additionally CW ESR allows us to measure the density of paramagnetic defects as well as the formation of higher F-center aggregates, lithium and impurity colloids during annealing experiments. The latest results will be presented.

[1] M. Ditter, H. Stork, B. Schuster, F. Fujara: Journal of Magnetic Resonance 209 (2011) 47-52

CPP 8.4 Mon 17:30 Poster C

Scanning force microscopy and polarized confocal-RAMAN microscopy for in-situ characterization of uniaxially stretched ethylene based thermoplastic elastomers — ●JÖRG MÜHLBÖCK, KRISZTINA VINCZE-MINYA, and SABINE HILD — Institute of Polymer Science, Johannes Kepler University, Linz, Austria

Polyethylene based elastomers are low crystalline materials which show interesting elastic mechanical behavior due to physical crosslinking. Nevertheless, the morphology of these polymers is still sparsely resolved. For a better understanding of the unique mechanical properties, microscopic changes in morphology and strain-induced variation in chain orientation of two polyethylenes with statistically distributed octene or butene side chains were monitored during uniaxial stretching using scanning force microscopy (SFM) and polarized Raman microscopy. For these purpose a stretching device has been developed and integrated in an existing SFM to visualize differences between an unstretched and stretched sample. Additionally, the set-up will be used to determine crystallinity and orientation of the samples before and after deformation via polarized Raman microscopy and polymer chain orientations were calculated for quantitative analysis. The correlation between the orientation, the arrangements of the amorphous and crystalline phases and the mechanical properties of the material at different elongation ratios allowed an interpretation of the macroscopic behavior on the microscopic scale.

CPP 8.5 Mon 17:30 Poster C

Border Search - Robust potential energy surface mapping technique — ●PROKOP HAPALA and PAVEL JELINEK — Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10, Prague, 16253, Czech Republic

Mapping of Potential Energy Surface (PES), searching for local and global minima of atomistic systems or paths with minimal energy barrier between these local minima is a long term goal of computational chemistry and material science. We propose novel robust method inspired by Metadynamics [1] providing advantages in several aspects: (a) No force evaluation is needed. (b) Positions in configuration space are sampled systematically and homogeneously. (c) Method setup has less parameters and is easier to control. (d) Lowest energy barrier is always found. (e) Number of PES evaluations required to reliable exploration of lowest energy path to neighboring local minimum is reduced by prohibiting re-examination of the same area.

[1] B. Ensing, et. al. Metadynamics as a tool for exploring free energy landscapes of chemical reactions. Acc. Chem. Res., 39, 73-81 (2006).

CPP 8.6 Mon 17:30 Poster C

Determination of the Modulation Transfer Function in a Holographic 2D-Data Storage System — ●CHRISTOPH MEICHNER¹, LOTHAR KADOR¹, CHRISTIAN PROBST², and HANS-WERNER SCHMIDT² — ¹University of Bayreuth, Institute of Physics and Bayreuther Institut für Makromolekülforschung (BIMF), 95440 Bayreuth, Germany — ²University of Bayreuth, Macromolecular Chemistry I and Bayreuther Institut für Makromolekülforschung (BIMF), 95440 Bayreuth, Germany

A holographic storage set-up was improved and characterized which is able to inscribe entire data pages into azobenzene-based media by means of a spatial light modulator (SLM). For the quantitative characterization of the imaging quality a fast and reliable method is required, which does not need every digital bit to be read out. To this end a simple measurement was performed which is based on the determination of the contrast of different periodical structures displayed on the SLM. The change in contrast of sinusoidal intensity patterns transferred through the optical system is analyzed with the hologram read-out camera in two directions perpendicular to the optical axis. The contrast as a function of the spatial frequency displayed on the SLM provides the data to calculate the modulation transfer function of the system. The experiments demonstrate the optical limitations of the set-up and the degree by which they are affected by the storage medium. In this way they yield information about the amount of storable data which is one of the key quantities in holographic data storage.

CPP 8.7 Mon 17:30 Poster C

Applications of Infrared Transition Moment Orientational Analysis (IR-TMOA) — ●WILHELM KOSSACK¹, WYCLIFFE KIPROP KIPNUSU¹, PERIKLIS PAPADOPOULOS², MALGORZATA JASIURKOWSKA³, and FRIEDRICH KREMER¹ — ¹Universität Leipzig, Fakultät für Physik und Geowissenschaften, Abteilung Molekülphysik, Linnestr. 5, 04103 Leipzig, Germany — ²Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55021 Mainz, Germany — ³The Henryk Niewodniczanski Institute of Nuclear Physics, Polish Academy of Sciences, Krakow, Poland

IR-TMOA is a recently developed experimental technique that enables one to determine the full *three dimensional* molecular order parameter tensor with respect to a sample coordinate system (reflecting degree of order and mean orientation directions). Relying on the dependence of the IR spectra on polarization *and* an intentional inclination of the sample with respect to the optical axis, specific information for the various molecular moieties in any IR translucent material can be obtained. The approach is of fundamental interest in polymer science and industry¹, for liquid crystal applications^{2,3}, organic electrets and it can provide insight into interactions in confined geometries^{2,4}. We will present examples from each of these fields emphasizing the multiple opportunities of this technique.

¹ Kossack, W. et al. *Polymer* 52, 6061 (2011). ² Jasiurkowska, M., W. Kossack et al. *Soft Matter* 8, 5194 (2012). ³ Kossack, W. et al. *Macromolecules* 43, 7532 (2010). ⁴ Kipnusu, W. K., W. Kossack et al. *Zeitschrift für Physikalische Chemie* 226, 797 (2012).

CPP 8.8 Mon 17:30 Poster C

Dynamic SEM image analysis of vibrating cantilevers (I) — ●MARIA-ASTRID SCHRÖTER¹, MATTHIAS HOLSCHNEIDER², CHRISTIANE WEIMANN¹, MARTIN RITTER³, and HEINZ STURM¹ — ¹BAM 6.9, Federal Inst. Materials Research, Berlin — ²Inst. Mathematics, Univ. Potsdam — ³Electron Microscopy TU Hamburg-Harburg

SFM cantilevers excited to vibration are used to perform intermittent- or non-contact modes or serve in force modulation techniques and derivatives thereof. Even sub-atomic resolution was demonstrated already. Advanced techniques include multi-frequency excitation for the use of higher modes to improve sensitivity or to examine tip-sample interactions related to materials properties. In all methods, non-linear effects can appear giving rise to harmonics of excitation frequency. The technique presented here named Dynamic Scanning Electron Microscopy (DySEM) enables us to image shapes of vibrating structures in different modes in terms of amplitude and phase shift measured by a lock-in amplifier (1,2). Our contribution concentrates on experimental issues and in this is part (I) the method is introduced and pictures of different modes and harmonics are presented. For the first time, the resulting motion induced by multiple frequency excitation (f_1 , f_2) is imaged at the sum (f_1+f_2) and difference (f_1-f_2) frequency. The mathematical analysis and a new developed model is presented in a second poster (II).

- (1) Schröter, Holschneider, Sturm; Nanotechn. 23, 435501 (2012).
 (2) Sturm, Schröter, Weimann; Microelectr. Eng. 98, 492 (2012).

CPP 8.9 Mon 17:30 Poster C

Dynamic SEM image analysis of vibrating cantilevers (II) — ●MARIA-ASTRID SCHRÖTER¹, MATTHIAS HOLSCHNEIDER², CHRISTIANE WEIMANN¹, MARTIN RITTER³, and HEINZ STURM¹ — ¹BAM 6.9, Federal Inst. Materials Research, Berlin — ²Inst. Mathematics,

Univ. Potsdam — ³Electron Microscopy TU Hamburg-Harburg

Dynamic Scanning Electron Microscopy (DySEM) is used to examine vibration modes and their harmonics at flexural and torsional resonance (1). In this part (II), the mathematical analysis of the imaging mechanism of DySEM is explained in detail. Recently, we presented a new model (2) describing the dynamic interaction of an electron beam with a periodically vibrating cantilever to explain and reproduce the topological features of amplitude images. Here we present an extended model taking into account the full periodic space-time dynamics i.e., amplitudes (moduli) and phase shifts as well as real and imaginary parts. A general methodology is demonstrated to distinguish non-linear features caused by the imaging process from those caused by cantilever motion. To describe complex dynamic contact behaviour, signal amplification is needed to enable measurements with a resolution below 10 nanometres. Strategies to improve image quality and sensitivity are discussed.

- (1) Sturm, Schröter, Weimann; Microelectr. Eng. 98, 492 (2012).
 (2) Schröter, Holschneider, Sturm; Nanotechn. 23, 435501 (2012).

CPP 8.10 Mon 17:30 Poster C

V16/VSANS - a new tool for soft matter research at the HZB — ●MIRIAM SIEBENBÜRGER, DANIEL CLEMENS, and KARSTEN VOGTT — Helmholtz Zentrum Berlin, Berlin, Deutschland

We would like to present the possibilities of the Time of Flight Small Angle Neutron Scattering beamline of the HZB, regarding the q-range, resolution and sample environment. Due to the use of different choppers, the q-range and resolution can be varied. First measurements of Soft Matter samples (colloids, polymers and proteins) will illustrate the performance of the VSANS. Furthermore, the available sample environments will be presented: a temperature controlled multi-sample holder, a sample cell with a very accurate temperature stability and a Rheo-SANS environment.

CPP 8.11 Mon 17:30 Poster C

The multipurpose hard x-ray beamline BL9 at DELTA — ●THOMAS BÜNING, MICHAEL PAULUS, CHRISTIAN STERNEMANN, and METIN TOLAN — Fakultät Physik / DELTA, Technische Universität Dortmund, D-44221 Dortmund

The hard x-ray beamline BL9 is located at the synchrotron radiation facility DELTA (Technische Universität Dortmund). Here, x-ray scattering studies can be performed using radiation in the energy range 4 - 30 keV provided by a superconducting asymmetric wiggler. The x-rays are monochromatized by a sagittally focusing Si (311) double crystal monochromator and the experimental endstation is equipped with a Huber six-circle diffractometer. At the beamline several detection schemes are available using point detectors, a MAR345 image plate scanner, or Pilatus 100 K area detector allowing for various x-ray scattering experiments such as (grazing incidence) x-ray diffraction, x-ray reflectivity, and small angle x-ray scattering. The beamline layout will be presented and different experiments will be discussed to emphasize the capabilities of the instrument.

CPP 8.12 Mon 17:30 Poster C

Microfluidics and microGISAXS - nanoscopic in situ characterization at the solid-liquid interface — ●VOLKER KÖRSTGENS¹, MARTINE PHILIPP¹, STEPHAN V. ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany — ²HASYLAB at DESY, 22603 Hamburg, Germany

We present an experimental microfluidic technique which allows for versatile structural investigations at the solid-liquid interface with high time resolution. In our approach reflection geometry using GISAXS (grazing incidence small angle x-ray scattering) is combined with a special designed microfluidic cell where the nanostructures at the solid-liquid interface are investigated. With the microfocussing of the highly brilliant x-ray beam of a third generation synchrotron source the kinetics of different processes in the nanoscopic regime are accessible. Applications include the investigation of attachment processes as in the layer formation of nanoparticles, detachment processes of unwanted detrimental films, as well as mixing and swelling experiments. Details on how to adjust the experimental settings (e.g. the beamsize) to the respective addressed questions will be given.

This work has been financially supported by the BMBF (grant num-

ber 05K10WOA).

CPP 8.13 Mon 17:30 Poster C

First-principles calculation of non-adiabatic coupling vector — PAVEL JELINEK¹, ENRIQUE ABAD², VLADIMÍR ZOBAC¹, PROKOP HAPALA¹, JAMES LEWIS³, and JOSÉ ORTEGA² — ¹Institute of Physics of the Czech Academy of Science, Prague, Czech Republic — ²Universidad Autónoma de Madrid, Madrid, Spain — ³West Virginia University, Morgantown, United States

Many of the chemical reactions and physical phenomena going beyond the Born-Oppenheimer approximation (B-O) are not possible to describe by conventionally first principles Molecular dynamics (MD) within (B-O) approximation. These phenomena need to describe not only ground state potential energy surface (PES), but also the excited one. The central quantity of such simulations is nonadiabatic-coupling vector (NAC), which allow us to describe correctly MD of the excited states.

The direct calculation of NAC based on local-orbital density functional theory has been recently implemented into Firaball code [1] together with time dependent Kohn-Sham dynamics within fewest switches surface hopping approximation [2,3]. Here we describe computationally efficient algorithm. We will present several cases of studies to demonstrate applications of this technique.

[1] J.P. Lewis et al, Phys. Stat. Sol. B, 248, 1989 (2011) [2] J. C. Tully, J. Chem. Phys. 93, 1061 (1990); C.F. Craig et al, Phys. Rev. Lett. 95, 163001 (2005). [3] N. L. Doltsinis. in John von Neumann Institute for Computing (NIC) Series (ed. J. Grotendorst, D. M., and A. Muramatsu) 377-397 (2002).

CPP 8.14 Mon 17:30 Poster C

a cold chopper spectrometer for ESS — LUCA SILVI^{1,2}, WIEBKE LOHSTROH^{1,2}, GIOVANNA SIMEONI^{1,2}, JÜRGEN NEUHAUS^{1,2}, and WINFRIED PETRY^{1,2} — ¹Technische Universität München - Physik Department E13 — ²Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II)

The European Spallation Source (ESS) will provide a high neutron flux, comparable to the best existing steady state reactors. The proposed cold direct time-of-flight spectrometer is a versatile instrument to address important scientific cases, ranging from soft matter and biological samples to magnetic and functional materials. These materials show motions on different length and time scales, requiring an instrument with flexible to high energy resolution and a broad accessible q -range. With the maximum pulse length of $1000\mu\text{s}$ (FWHM) usable for a clean resolution function, an energy resolution of $100\mu\text{eV}$ at 5Å is expected, with the possibility to reach $5 - 10\mu\text{eV}$ at 9Å . The natural bandwidth usable for any experiment in Rate Repetition Multiplication (RRM) mode is 2.6Å , covering a reasonable part of $S(\mathbf{q}, \omega)$ in one measurement. The chopper and guide system of proposed instrument will be optimized for cold neutrons and will foresee the use of dedicated sample environments (polarization analysis, magnetic fields).

CPP 8.15 Mon 17:30 Poster C

Bispectral powder diffraction at the long pulse source ESS — NICOLÒ VIOLINI¹, WERNER SCHWEIKA^{1,2}, ANDREAS HOUBEN³, KLAUS LIEUTENANT⁴, and PAUL F. HENRY² — ¹JCNS, Forschungszentrum Jülich GmbH, D-52425 Jülich Germany — ²European Spallation Source ESS AB, Lund, Sweden — ³RWTH Aachen University, Germany — ⁴Helmholtz-Centre Berlin, Germany

Within the ESS Design Update Program, funded by the German Federal Ministry of Education and Research, we investigate a versatile instrument concept for powder diffraction at the ESS. Typical applications will be the determination of structures involving light or neighboring elements, complex magnetic structures, and the ability to *in-situ* follow phase transitions in reactive or functional materials, under conditions close to operation. To match the various needs, we investigate a bispectral time-of-flight diffractometer that efficiently makes use of thermal and cold neutrons ($0.8\text{-}4.6\text{Å}$). Moreover a wide wavelength spectrum is of interest to exploit the backscattering option with high resolution. The conceptual design utilizes a $10\times 10\text{mm}^2$ eye-of-the-needle[1] at 6m from the source, defining an image of 5 to 10 mm diameter with an initial divergence of $\pm 0.6^\circ$. It reduces background by more than two orders of magnitude, as early as possible, thus it helps to design more cost-efficient shielding. It allows to fit in counter rotating disc choppers that are able to provide flexible resolution from $10\mu\text{s}$ to 1 ms. The desired phase space is transported by elliptic guides to the sample position of similar size, with only small losses. [1] A. Houben et al., NIMA, 2012, 680, 124.

CPP 8.16 Mon 17:30 Poster C

Perspectives for spectroscopy at the future European Spallation Source — NICOLÒ VIOLINI, JÖRG VOIGT, THOMAS BRÜCKEL, EARL BABCOCK, and ZAHIR SALHI — Jülich Centre for Neutron Science, JCNS, Forschungszentrum Jülich GmbH, ESS Design Update Program - Germany, D-52425 Jülich Germany

Within the ESS Design Update Program funded by the German Federal ministry of Education and Research, we investigate the performance of a multispectral time-of-flight spectrometer at the long pulse source of the ESS, which promises the applicability to a wide manifold of scientific activities of research: strongly correlated electron materials, disordered systems, functional materials, magnetism, soft-matter and biophysics. The concept makes use of a pin-hole $2.5\times 4.5\text{cm}^2$ at 6m from the moderator that helps to reduce the background. A powerful double elliptic guide system is able to transport neutron brilliance to a small sample size $1\times 3\text{cm}^2$, with a brilliance transfer approaching 1. The chopper system contains fast choppers in the focal points of the ellipses providing unprecedented resolution or intensity depending on the request of the experiment. In combination with the band-width choppers and pulse suppression choppers, the system is perfectly adapted to the requirements of the novel repetition rate multiplication method. The use of polarization analysis for this instrument class is under investigation and its implications will be discussed during the talk.

CPP 9: Poster: Interfaces and Thin Films (joint session with DECHEMA and VDI)

Time: Monday 17:30–19:30

Location: Poster C

CPP 9.1 Mon 17:30 Poster C

Fabrication of nanostructured titania thin films for application in hybrid photovoltaics — WEIGUO LU, MARTIN A. NIEDERMEIER, GREGORY TAINTER, and PETER MÜLLER BUSCHBAUM — TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany

Nanostructuring of titanium dioxide thin films has been the subject of numerous studies over the last years due to their important role in various optoelectronic applications, e.g. photovoltaics. These thin films need to meet certain requirements. Exhibiting a high effective surface area and a decent degree of crystallinity is crucial for the functionality and performance. Using block-copolymer templates in combination with a sol-gel synthesis approach to produce metal oxide thin films gives a high control over the morphology and is a promising way to meet those requirements. In this study, nanostructured titania thin films are fabricated with a bi-continuous foam-like structure. The diblock-copolymer poly(styrene-block-ethylene oxide) is used as the templating agent in a sol-gel process to fabricate hybrid thin films, which are subsequently transferred to anatase titania films via a high-

temperature calcination step. Due to the hybrid nature of the thin films after the sol-gel preparation route, our films are even suitable for super-structuring. The morphology is investigated with imaging techniques like atomic force microscopy or scanning electron microscopy. The optical properties are probed with UV/Vis spectroscopy and white light interferometry.

CPP 9.2 Mon 17:30 Poster C

Microfabrication and characterization of stress-reduced YSZ membranes — FLORIAN KUHL¹, MARKUS PIECHOTKA¹, DANIEL REPPIN¹, TORSTEN HENNING¹, JÜRGEN JANEK², and PETER J. KLAR¹ — ¹I. Physikalisches Institut, Justus Liebig University, Heinrich-Buff-Ring 16, DE-35392 Giessen, Germany — ²Physikalisch-Chemisches Institut, Justus Liebig University, Heinrich-Buff-Ring 58, DE-35392 Giessen, Germany

The oxygen conductor YSZ (yttria-stabilized-zirconia) is a material often used as the electrolyte in solid oxide fuel cells. To achieve a lower operation temperature and to maximize the currents it is necessary to miniaturize the fuel cell components, especially to reduce

the thickness of the solid electrolyte. Another application of very thin YSZ films may be their utilization as an ion source. We fabricated free-standing YSZ membranes by partially removing a Si substrate by anisotropic wet-chemical etching. We characterized the resulting inhomogeneous strain distribution and found a correlation between the size of the membranes and the strain induced pattern. Arrays of free-standing stress-reduced membranes with a high packing density were prepared by using cross-like masking patterns. Deposition of a porous Pt electrode onto the YSZ membranes allows the measurement of their ionic conductivities.

CPP 9.3 Mon 17:30 Poster C

Order and phase behavior of thin film of diblock copolymer-selective nanoparticle mixtures : A molecular dynamics simulation study — ●LENNI S. SHAGOLSEM^{1,2} and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden — ²Technische Universität Dresden

We study a coarse grained model of AB diblock-copolymer and nanoparticle mixtures confined between two identical walls in slit geometry. The nanoparticles are selective with respect to the A-block of the copolymer, while the walls are repulsive and non-selective with respect to both the copolymers and nanoparticles. We systematically explore the various equilibrium morphologies formed by the copolymer nanocomposites in this confined geometry, and construct the corresponding phase diagram in diblock composition and nanoparticle concentration space. We observe both vertically and horizontally oriented lamellar structures. The vertically oriented lamellae is formed by symmetric and slightly asymmetric diblock-copolymers at low nanoparticle concentrations and it has a very limited region of stability in the phase space, whereas the horizontal lamellae can be realized up to highly asymmetric diblock-copolymers and at high nanoparticle concentrations. The formation of horizontally oriented lamellae is driven by the chains (mainly nanoparticle repulsive B-blocks) to relax stretching near the confining surfaces. By considering the horizontal lamellae, we also investigate the effect of nanoparticle concentration on the lamellar layer thickness.

CPP 9.4 Mon 17:30 Poster C

Investigation of critical parameters of polymer adsorption for chains with different architecture — ●OLGA MIRONOVA^{1,2} and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany — ²TUD, Dresden, Germany

In order to understand the role of polymer chain architecture on adsorption properties, we used scaling arguments to analyze polymer systems. We suggest that molecules with the same molecular weight but with different structure can have different adsorption properties, such as critical energy of adsorption and crossover exponent. For such polymers this difference can be applied as basis in separation technique like Liquid Chromatography at Critical Condition. For computer simulation of polymer systems we used the Bond-Fluctuation Model (BFM). End-grafted polymers at an adsorbing surface are considered under good solvent conditions. We compared three types of polymer architecture: linear, star-shaped and hyper-branched. It was found that critical parameters for 4-arm star-shaped and linear polymers are very close to each other. We also studied competitive adsorption from a dilute solution containing a mixture of stars and linear polymers. For hyper-branched polymers we realized essential ensemble averages over many realizations of branching topology.

CPP 9.5 Mon 17:30 Poster C

Static and dynamic properties of cross-linked and non cross-linked polymer brushes. — MICHAEL LANG¹, MAX HOFFMANN², ●MARCO WERNER^{1,3}, and JENS-UWE SOMMER^{1,3} — ¹Leibniz-Institut für Polymerforschung Dresden, Germany — ²Universität Heidelberg, Germany — ³Technische Universität Dresden, Germany

We compare dense layers of surface-grafted polymer chains (polymer brushes) with and without additional random cross-links between the chains using the bond fluctuation model. In non cross-linked brushes with intermediate and low grafting densities, chain conformations can be described by random walks in a parabolic potential. Cross-linking leads to a reduction of brush height, whereby a large fraction of this reduction stems from cross-links between monomers of the same chains. Most cross-links between different chains do not contribute to a significant collapse of the brush, because they are established between monomers of similar contour distance to the grafting points, where the balance of stretching forces and chain elasticity stays almost unmodified by a cross-link. Chain dynamics of non cross-linked brushes

is dominated by arm retraction processes suggesting an exponential increase of relaxation time as function of chain length. The largely confined motion of non cross-linked grafted chains under a cross-linked brush highlights the recently discovered critical behavior [D. Romeis, H. Merlitz and J.-U. Sommer, J. Chem. Phys. 136 (2012) 044903] of monodisperse brushes as well as the dominance of arm retraction processes for the ultimate relaxation of the chains.

CPP 9.6 Mon 17:30 Poster C

Slippage of polymers: Influence of the chemical structure — ●MISCHA KLOS¹, SEBASTIAN BACKES¹, MATTHIAS LESSEL¹, OLIVER BÄUMCHEN², and KARIN JACOBS¹ — ¹Saarland University, Experimental Physics, 66041 Saarbruecken, Germany — ²Dept. of Physics & Astronomy McMaster University, Hamilton, ON, Canada

The continuing miniaturization of microfluidic devices causes a growing importance of the solid/liquid interface for the flow dynamics. Our experiments probe slippage using the dewetting process of thin polymer films on hydrophobic substrates [1]. As hydrophobic coatings, we use amorphous polymers (AF1600, AF2400) and different types of highly ordered self-assembled silane monolayers on top of ultraflat silicon substrates. On silane surfaces, polystyrene (PS) of low molecular weight exhibits slip lengths of several hundreds of nanometers up to even micrometers [2]. On AF1600, no significant slip is observable. Recent studies using scattering techniques showed an ordering effect of PS at the solid/liquid interface depending on the structure of the substrate [3]. Will the situation change if, instead of PS, other polymers like PMMA or PVP are used? In contrast to PS, PMMA has no phenyl rings. Moreover, we probe how the crystallinity of the substrate influences slippage: We show results of dewetting experiments supplemented with X-ray scattering methods to analyze the slippage mechanism at the solid/liquid interface. [1]O. Bäümchen et. al., J Phys Condens Matter, vol. 24, no. 32, pp. 325102, 2012 [2]R. Fetzer et. al., Europhys Lett, vol. 75, no. 4, pp. 638, 2006 [3]P. Gutfreund et al., arXiv.org, vol. cond-mat.soft. 2011

CPP 9.7 Mon 17:30 Poster C

Preparation conditions influence dewetting behavior of thin polymer films — ●MISCHA KLOS, MATTHIAS LESSEL, and KARIN JACOBS — Saarland University, Experimental Physics, 66041 Saarbruecken, Germany

Dewetting of thin polymer films on smooth substrates like silicon wafers can be influenced by many factors such as intrinsic material and surface parameters, the film itself and even the quality of the substrate. So the sample preparation is a crucial step in the entire experiment. Reliable results are only achieved by fully characterized systems, which implicates perfect cleaning. Silicon wafers are common substrates to study the flow dynamics of polymer film. Since they feature a very high surface energy, also dust, dirt, impurities or differences in the preparation procedure have an influence on the quality of the surfaces. Dust for example can act as a nucleation core on the one hand and on the other hand, depending on the density, it can stabilize the film due to pinning. We show a comparison of different preparation and cleaning methods for silicon surfaces and their impact on the stability of thin polystyrene films.

CPP 9.8 Mon 17:30 Poster C

Synthesis and ARXPS Investigations of Nitrile-Functionalized Ionic Liquid Systems — ●SANDRA KRICK CALDERÓN¹, INGA NIEDERMAIER¹, NICOLA TACCARDI², FLORIAN MAIER¹, PETER WASSERSCHIED², PETER LICENCE³, and HANS-PETER STEINRÜCK¹ — ¹Physikalische Chemie II — ²Chemische Reaktionstechnik, Egerlandstr. 3, 91058 Erlangen — ³School of Chemistry, Nottingham NG7 2RD

Due to their outstanding physicochemical properties, ionic liquids (ILs) are promising candidates for many catalytic applications. One remaining challenge is the dissolution of transition metal complex (TMC) catalysts in ILs. Groups such as nitriles facilitate the interaction between IL and TMC up to direct IL-TMC complex formation. Two new nitrile-functionalized ILs ($[(C_4CN)MIM][OTf]$ and $[(C_4CN)_2IM][OTf]$) were successfully synthesized. Additionally, two palladium-based nitrile-coordinated complexes ($[(C_4CN)MIM_2PdCl_2][OTf]_2$ and $[-(C_4CN)-IM(C_4CN)-PdCl_2]_x[OTf]_x$) were prepared from these ILs. Angle-resolved X-ray photoelectron spectroscopy (ARXPS) revealed a sandwich-like structure for $[(C_4CN)MIM][OTf]$ at the IL/vacuum interface, with the anion enriched in the outermost layer and the cation located below. Contrary, $[(C_4CN)_2IM][OTf]$ shows a uniform distribution at the surface. In both cases, the CF_3 moiety of the $[OTf]^-$

anion is pointing towards vacuum. Quantitative analysis of the XPS data of both metal-IL-complexes show a loss in anion which leads to the assumption that a carbene complex is formed. Supported by the DFG through SPP 1191 and by the EAM Cluster of Excellence.

CPP 9.9 Mon 17:30 Poster C

Unusual water uptake in ultrathin polyvinyl acetate films — ●HEIKO HUTH and CHRISTOPH SCHICK — Universität Rostock, Institut für Physik, Wismarsche Str. 43-45, 18051 Rostock, Germany

The water sorption of polyvinyl acetate (PVAc) at different relative humidity for bulk like and ultra-thin films was studied by AC chip calorimetry. For a micrometer sized sample of about 200 ng the plasticizing effect of water vapor is the same as in conventional differential scanning calorimetry (DSC) employing mg samples with closed volume and well defined water content of the mg scale samples is found. With decreasing film thickness the water sorption behavior becomes more complex and an increasing amount of adsorpt excess water is observed. The effect can be discussed as a water layer on top and below the polymeric film dependent on the surface properties of the underlying sensor surface. For the experiments a new setup to measure heat capacity of thin film samples under controlled humidity was developed. The AC chip calorimeter uses a self-made humidity generator applying mass flow controllers. A quartz crystal microbalance (QCM) allows checking the mass change during water uptake. The technical details of the device and the extensions for humidity control are discussed too.

CPP 9.10 Mon 17:30 Poster C

Characterization and investigation of the diffusion of silver nanoparticles using single molecule fluorescence spectroscopy — ●MARTIN HARTMANN, STEFAN KRAUSE, THOMAS BAUMGÄRTEL, and CHRISTIAN VON BORCZYKOWSKI — Optical Spectroscopy and Molecular Physics Group, Chemnitz University of Technology, 09126 Chemnitz, Germany

Optical properties like the absorption or emission behavior of silver nanoparticles as a function of the particle size have been extensively studied in the past. Furthermore the catalytic and optical surface enhanced properties are of special interest.

In our experiments small silver nanoparticles with a diameter below 1 nm showed surprisingly diffusion phenomena on a pure silicon dioxide surface. The aim of this work is to characterize those nanoparticles, to find a reason why they are diffusing and to investigate their diffusion. Experiments were performed by means of optical microscopy and atomic force microscopy. We are able to show, that the investigated particles consist of less than 22 silver atoms. The reason for the diffusion seems to be a small water film on the silicon dioxide surface. Diffusion measurements for different humidities of the surrounding atmosphere have been carried out. It turned out that three main diffusion coefficients exist and two of them depend on the air humidity.

CPP 9.11 Mon 17:30 Poster C

Adsorption Behavior of Catanionic Surfactant Mixtures at the air/liquid interface — ●MARTIN UHLIG, HEIKO FAUSER, and REGINE V. KLITZING — Stranski-Laboratorium, Department of Chemistry, TU Berlin, Straße des 17. Juni 124 D-10623 Berlin, Germany

The strong synergism of catanionic surfactant mixtures is known for a long time. The synergism allows to reduce the expended amount of surfactant, thus making catanionic surfactant mixtures eco-friendly. Therefore, these mixtures are of great interest for a broad field of applications. However, only very recently basic research was performed about the stability of foams formed with these mixtures. It was shown that the formation of surface active complexes and aggregates strongly enhances the adsorption at liquid-air interfaces and thus the foamstability [1].

Literature also shows that mixtures of surfactants with unequal chain length differ in surface properties in comparison to mixtures with equal chain length [2]. Hence, the focus of our work is on the influence of the surfactant alkyl chain length on the foam properties. We investigate catanionic mixtures from two common surfactant types, sodium alkyl sulfates and quaternary alkylammonium bromides. Both surface tension and the surface elasticity of mixtures with both matching chain length and mismatching chain length are investigated. Studies about the correlation between adsorbed amount of surfactants, interactions in thin foam films, foamability and foam stability are in progress.

[1] Varade, D. et.al.; *Soft Matter*, 2011, 7, 6557-6570

[2] Patist, A. et.al.; *Langmuir*, 1997, 13, 432-434

CPP 9.12 Mon 17:30 Poster C

Controlling probe dynamics by modification of adsorption site density in confined liquids — DANIELA TÄUBER, ●FABIAN MEIER, and CHRISTIAN VON BORCZYKOWSKI — nanoMA, TU-Chemnitz, Institut für Physik

The mobility of probe molecules in confined liquids is influenced by short adsorption events at the interface. Here we report about the modification of the surface silanol density at silica substrates and its effect on single dye dynamics in ultrathin liquid films. In contrast to ensemble methods, single molecule microscopy provides information on a local scale with sub-micron resolution. Thereby, probability distributions of diffusivities (scaled square displacements at fixed time lags) yield additional details to the conventional analysis of particle tracking via calculation of mean square displacements along detected trajectories. The probe diffusion in ultrathin liquid films can be modeled by a two layer system, consisting of a heterogeneous near surface layer with slowed diffusion on silanol patches and a homogeneous upper layer[1]. Single molecule tracking experiments on substrates with modified surface silanol density are compared to simulations. High adsorption site density combined with two-dimensional confinement in mesopores allows us to use adsorbed dye molecules as probes for the dynamics of the liquid in such pores.

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

CPP 9.13 Mon 17:30 Poster C

Mechanism analysis of symmetric adhesion of water-swelling polymer films — ●RINA IKUBO, MARKUS SCHINDLER, and PETER MÜLLER-BUSCHBAUM — TU München, Physik Department, LS Funktionelle Materialien, James-Frank-Str.1, 85748 Garching, Germany

Commonly symmetric adhesion between polymer films is studied in case of hydrophobic polymers. The symmetric adhesion of polymer films which swell in water, which ubiquitously exist around our atmosphere, is less investigated despite its technological importance and scientific interest. Previous studies on our model system consisting of the statistical copolymer poly(ethylhexylacrylate-stat-methylmethacrylate) have shown that the two components of the polymer establish an enrichment layer of methylmethacrylate(MMA) at the top surface, and the MMA content changes depending on the relative humidity. PMMA is also studied as the polymer film which swells in water. We present a study on the influence of water on the internal reorganization of adhesive films that include PMMA as one component, its behavior on symmetric adhesion and discuss the effect of hydration on the surface composition and entanglement of surface molecules.

CPP 9.14 Mon 17:30 Poster C

Combination of grafted and adsorbed polymer chains on solid surface for the creation of multicompartamental responsive coatings — ●SAMANTHA MICCIULLA and REGINE VON KLITZING — Stranski-Lab für Physikalische u. Teoretische Chemie, Technische Universität Berlin, Germany

Responsive coatings are of interest for a large number of researchers due to their applicability as highly tunable release systems. Functionality and structural properties allow for the creation of systems which respond to many different stimuli, like pH, temperature, ionic strength and light. The combination of grafted and physisorbed blocks in an unique matrix has been object of studies in the last few years. The design of such coatings arises fundamental questions, for instance which materials and geometries can be successfully combined, which properties are induced from the complex assembly and how the responsiveness is consequently affected. Task of our study is to clarify the mentioned aspects. The system under investigation is prepared by grafting thermoresponsive polymers on silica surface, which is used as macroinitiator for the growth of a strong polyelectrolyte block, onto which polyelectrolyte multilayers are adsorbed. The "grafting from" performed by Surface Initiated Atom Transfer Radical Polymerization allows for controlled chain growth and low polydispersity. The adsorption is performed by dipping the substrate in oppositely charged polyelectrolyte solutions. Sample characterization is carried out by combining Ellipsometry, Atomic Force Microscopy, Contact angle and X-Rays Reflectometry, while responsive properties are monitored by Ellipsometry.

CPP 9.15 Mon 17:30 Poster C

Improvement of the lamellar structure in block copolymer

thin films by solvent vapor treatment — ALESSANDRO SEPE¹, DORTHE POSSELT², KASPER SWIATEK², JIANQI ZHANG¹, SEBASTIAN JAKSCH¹, RICHARD STEINACHER¹, JAN PERLICH³, DETLEF-M. SMILGIES⁴, and CHRISTINE M. PAPADAKIS¹ — ¹TU München, Physik-Department, Physik weicher Materie, Garching — ²IMFUFA, Department of Science, Systems and Models, Roskilde University, Denmark — ³HASYLAB at DESY, Hamburg — ⁴Cornell High Energy Synchrotron Source, Cornell University, Ithaca NY, USA

Defects in nanostructured block copolymer thin films are often annealed by solvent vapor treatment. We have studied the structural ordering in lamellar poly(styrene-*b*-butadiene) thin films during exposure to cyclohexane vapour and subsequent drying using X-ray reflectometry and in-situ, real-time grazing-incidence small-angle X-ray scattering [1]. The films had initially the parallel lamellar orientation and were subject to two swelling/drying cycles. We found that the lamellar order after this treatment is best when (i) a well-correlated parallel lamellar orientation is obtained during the first swelling cycle and (ii) when the film is dried at a sufficiently slow rate.

1. Z. Di, D. Posselt, D.-M. Smilgies, C.M. Papadakis, *Macromolecules* **43**, 418 (2010).

2. Z. Di, D. Posselt, D.-M. Smilgies, C.M. Papadakis et al., *Macromolecules* **45**, 5185 (2012).

CPP 9.16 Mon 17:30 Poster C

Molecular motions of confined ultra-thin polystyrene films studied by REDLS — FAN-YEN LIN, TASSILO KAULE, RÜDIGER BERGER, HANS-JÜRGEN BUTT, and WERNER STEFFEN — Max Planck Institute for Polymer Research, P.O. Box 3148, 55128 Mainz, Germany

Resonance Enhancement Dynamic Light Scattering, REDLS*, is used to probe the surface and interface dynamics of (immiscible) polymers in double-layers. A low T_g (53°C) Polystyrene (PS) is supported by a gold layer and covered by a solid, transparent, high T_g (> 200°C) Polynorbornene (PN) layer polymerized onto the PS layer directly. We observe two Arrhenius-like processes above and below the bulk T_g. The degree of confinement is influenced partly by the thickness of the capping layer. The surface dynamics going from a free PS surface to confined is strongly changed.

*Plum M. A., Menges B., Fytas G., Butt H. J., Steffen W., Rev. Sci. Inst. 2011, 82, (1), 15102

CPP 9.17 Mon 17:30 Poster C

Interaction of Ta and Nb based salts with ionic liquids — STEFAN KRISCHOK¹, ADRIANA ISPAS¹, ANDRÉ ZÜHLSDORFF¹, ANGELA ULBRICH¹, ANDREAS BUND¹, and FRANK ENDRES² — ¹Technische Universität Ilmenau, Institut für Mikro- und Nanotechnologien, 98693 Ilmenau, Germany — ²Clausthal University of Technology, Institute of Electrochemistry, 38678 Clausthal-Zellerfeld, Germany

We have analyzed the changes of the surface properties of the ionic liquids (ILs) 1-butyl 1-methyl-pyrrolidinium bis(trifluoromethylsulfonyl)amide ([BMP][TFSA]) and 1-methyl-3-propyl imidazolium bis(trifluoromethylsulfonyl)amide ([PMIm][TFSA]) with and without dissolved NbF₅ and TaF₅ by X-ray photoelectron spectroscopy (XPS). The relative intensities of core level emission agree very well with the expected stoichiometry. Moreover, the observed chemical shifts are in agreement with the chemical structure. Upon solution of the salts the situation changes drastically. In particular a strong modification of the cation/anion ratio is observed. With increasing amounts of TaF₅ and NbF₅ both, the Ta or Nb concentration and the cation anion ratio increases in the near surface region. Additionally a new salt induced F component appears in the XPS spectra. The detected TaF₅ (NbF₅) concentration in comparison to the nominal volume concentration and the correlation with the observed [TFSA] depletion in the surface region will be discussed in more detail. Finally, results on more complex metal salts will be presented. A fundamental understanding of the investigated interaction processes provides the basis for future studies on electrochemical processes in these systems.

CPP 9.18 Mon 17:30 Poster C

Influence of the Air/Water Interface on the Monolayer of Block Copolymers — CHRISTIAN APPEL, MARTIN KRASKA, and BERND STÜHN — Experimental Condensed Matters Physics, TU Darmstadt, Germany

Monolayers of special amphiphilic polymers are investigated in terms of compression behaviour and structure of the air/water (a/w) interface. We compare *bad/good* solvent conditions for two different

polymer systems and study the morphology at the interface in dependency on the ruling surface pressure. In one of the polymer systems a hydrophobic polymer (polybutylacrylate) is anchored to the interface by a hydrophilic oligomer (polyethylenglycol). We compare this system with the complementary situation, where a hydrophilic polymer (poly-2-vinylpyridine) is anchored by a hydrophobic oligomer (polyvinylferrocene).

We recorded compression isotherms and studied the structure of the monolayers by X-Ray reflectometry in situ at the a/w interface an ex situ by the preparation of LB-films. These experiments lead to detailed structural pictures of the monolayers. We observed in situ the forming of a two-layer system in dependency of the surface pressure. In the semi-dilute regime we treat the monolayer systems as quasi 2D and quantify the influence of the water surface in terms of 2D power laws, e.g. the interface acts as a *bad/good* solvent for the monolayers, respectively.

CPP 9.19 Mon 17:30 Poster C

Auxetic behaviour of α -polypropylene with crosshatch structure — MARTIN NEUMANN and ROBERT MAGERLE — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

Auxetic materials expand laterally when stretched. We have discovered this unusual behaviour in thin films of elastomeric polypropylene (ePP), a semi crystalline polymer with a low degree of crystallinity. The crystalline lamella are orientated perpendicular to the film plane and branch into daughter lamellae with branching angles of 80° forming a crosshatch structure. With a microtensile testing setup that allows for simultaneous imaging with atomic force microscopy (AFM) we measured series of AFM images during uniaxial elongation of a 1.75 μ m thick film. Approximately 10 μ m large patches of the crosshatch structure expand perpendicular to the stretching direction. This corresponds to a negative Poisson ratio of -0.2. AFM images taken after stepwise relaxation show, that the auxetic deformation is almost completely reversible. Our results show, that auxetic behaviour is an intrinsic property of α -polypropylene with crosshatch structure. The auxetic behaviour is explained with a model based on elongating lamella branches with fixed branching angles, fixed lamella width, and a conservation of crystalline volume.

CPP 9.20 Mon 17:30 Poster C

Ordering effects in thin xenon films studied with NMR — ALEXANDER POTZUWEIT, HAGEN ALLMRODT, LARS KRAFT, ANUSCHKA SCHAFFNER, and HEINZ JÄNSCH — Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg

We employ NMR of hyperpolarized ¹²⁹Xe to investigate ordering phenomena and diffusion in thin Xe films. To increase the sensitivity towards structurally caused inhomogeneities a small line width is favorable. In solid Xe the line width is dominated by dipolar interaction with neighboring nuclear spins. This can be substantially reduced by diluting the NMR-active isotope ¹²⁹Xe in the NMR-inactive isotope ¹³²Xe. Thus we are able to investigate ordering effects like annealing. Using different pulse sequences makes it possible to distinguish local and global effects. Here we present the technical development of the apparatus and discuss first results.

CPP 9.21 Mon 17:30 Poster C

Influence of strain and slip on the dewetting of thin films — ANDREAS REINDL^{1,2} and MARKUS RAUSCHER^{1,2} — ¹Max-Planck-Institut für Intelligente Systeme, Stuttgart — ²Institut für Theoretische Physik IV, Universität Stuttgart

Thin polymer films produced by spin coating techniques often exhibit residual strain. We investigate the influence of this strain on the stability for the case of weak hydrodynamic slip at the substrate surface and for the case of strong slip (plug flow limit), i.e., we address the question whether a film dewets or not. The linear stability analysis of the corresponding thin film equations shows that for weak slip, residual strain does not destabilize the film. In the case of strong slip, however, sufficiently large residual strain can lead to dewetting of the film.

CPP 9.22 Mon 17:30 Poster C

Real-time studies on annealing of Tetratetracontane (TTC) by X-Ray diffraction — LINUS PITHAN¹, ANDREAS OPITZ¹, ALEXANDER HINDERHOFER², EDUARD MEISTER³, CHRISTIAN FRANK², MICHAEL KRAUS³, WOLFGANG BRÜTTING³, FRANK SCHREIBER², and STEFAN KOWARIK¹ — ¹Humboldt Universität Berlin — ²Universität Tübingen — ³Universität Augsburg

TTC ($C_{44}H_{90}$) is e.g. used as dielectric interlayer in organic field-effect transistors [1]. For such devices large molecular grains with smooth surfaces are crucial. Here we report real time grazing incidence X-Ray diffraction (GIXD) measurements monitoring the annealing process of TTC thin films on silicon dioxide previously deposited by vapor deposition. Furthermore atomic force microscopy (AFM) and X-Ray reflectivity (XRR) results are presented. We find that randomly oriented and lying molecules on the surface rearrange into standing up molecules and fill subjacent layers [2]. By AFM measurements it can be shown that islands of molecules form large terraces in the annealing process.

[1] Kraus et al.; *Organic Electronics*, 12, 5, May 2011, 731-735, DOI:10.1016/j.orgel.2011.02.001

[2] Weber et al.; *J. Chem. Phys.* 136, 204709 (2012), DOI:10.1063/1.4719530

CPP 9.23 Mon 17:30 Poster C

The effect of salt ions on the protein adsorption at lipid membranes — ●HOLGER GÖHRING, MICHAEL PAULUS, and METIN TOLAN — Fakultät Physik/DELTA, Technische Universität Dortmund, D-44221 Dortmund

Lipid membranes serve in biological cells as boundaries between the intracellular and extracellular region. Many biological transport processes taking place at membranes are associated with the adsorption of proteins. Here the investigation of protein - membrane interactions is crucial for a deeper understanding of such processes. In the case of electrostatic interaction the screening effect of salt ions can be used to control the adsorption. The presented study investigates the protein adsorption to Langmuir films under the presence of different concentrations of salt ions. Langmuir films prepared on a liquid subphase are an ideal model for cell membranes. By varying the salt concentrations the electrostatic interaction between the films and proteins is altered. However, also the accumulation of ions at the Langmuir films has to be taken into account just as the different impact of the salts on the stability of the proteins. To regard those effects different salt ions are used during this study. The adsorption process is investigated by x-ray reflectivity (XRR) measurements, which allow the determination of the electron densities of thin layers at the liquid surface.

CPP 9.24 Mon 17:30 Poster C

Effects of Reactive Oxygen Species on Phosphatidylglycerol Monolayer with Adsorbed Polyethylenimine — ●ANDREAS GRÖNING¹, HEIKO AHRENS¹, FRANK LAWRENZ¹, THOMAS ORTMANN¹, FRITZ SCHOLZ², and CHRISTIANE A. HELM¹ — ¹Inst. für Physik, Uni Greifswald, Felix-Hausdorff-Str. 6, D-17487 Greifswald — ²Inst. für Biochemie, Uni Greifswald, D- 17487 Greifswald

Polymer adsorption is widely used to modify surfaces. To investigate the protective effect against free oxygen radicals polyethylenimine (PEI) is adsorbed onto oppositely charged DMPG lipid monolayers at the air/water interface. The structure of the lipid-polyelectrolyte system is investigated with X-ray reflectivity and grazing incidence diffraction. At different pH-values and mixed with a variety of salts PEI adsorbs flatly (2.8 nm). But in the presence of Fe(II)SO₄ and EDTA in the solution a 15nm thick PEI layer is formed due to incorporation of Fe²⁺ EDTA complexes. Radical oxygen species are produced via the Fenton's reaction. The reaction is started by H₂O₂ injection. If a highly compressed monolayer is attacked, the lateral pressure is reduced by 10mN/m within 30min for thin and 3h for thick adsorbed PEI layers. With X-ray reflectivity it is observed that the PEI layer shrinks and eventually disappears. Simultaneously, Fe²⁺ binds to the lipid monolayer and the solid lipid phase changes from NN-tilted to hexagonal.

CPP 9.25 Mon 17:30 Poster C

Fabrication of carbon nanomembranes by helium ion beam lithography — ●XIANGHUI ZHANG, HENNING VIEKER, ANDRÉ BEYER, and ARMIN GÖLZHÄUSER — Fakultät für Physik, Universität Bielefeld, Postfach 10 01 31, 33501 Bielefeld, Germany

The scanning helium ion microscope (HIM) has been recently employed as an imaging and metrology tool for nanotechnology. In addition, the helium ion beam is capable of creating nano-sized patterns and performing nanofabrication as commonly done in a focused ion beam (FIB) system. It is known that aromatic self-assembled monolayers (SAMs) can be cross-linked due to electron irradiation and form mechanically stable carbon nanomembranes (CNMs). Here we use a helium ion beam as direct writing tool to cross-link 4'-nitro-1,1'-biphenyl-4-thiol (NBPT) SAMs with arbitrary patterns. The cross-linked SAMs

were transferred to either silicon substrates with an oxide layer or transmission electron microscopy (TEM) grids for further characterizations or applications. After being transferred, the evolution of SAM's crosslinking process could be investigated by the HIM imaging. Formation of wormlike morphology with preferential directions indicates that the crosslinking starts from the energetically favorable sites, such as molecular domains with certain crystalline orientation. Furthermore, we also use the ion beam to form nanopores in the CNM with an attainable feature size of 5 nm.

CPP 9.26 Mon 17:30 Poster C

Interdiffusion within polyelectrolyte multilayers: influence of kind and weight of polycation and the design of diffusion barriers — ●MALTE PASSVOGEL¹, PETER NESTLER¹, RALF KÖHLER², and CHRISTIANE A. HELM¹ — ¹Inst. für Physik, Uni Greifswald, D-17487 Greifswald — ²Helmholtz-Zentrum für Materialien und Energie, D-14109 Berlin

With neutron reflectivity the position and width of the internal interface between protonated and deuterated blocks of polyelectrolyte multilayers is determined. First, a standard system formed from PDADMA and PSS (protonated or deuterated) in 0.1M NaCl solution is investigated. Immersion in a concentrated salt solution (1M NaCl) for different annealing times shows interdiffusion. The diffusion constant depends non-linearly on the PDADMA molecular weight. This finding suggests that the diffusing entities are polycation/polyanion complexes. For large PDADMA molecular weight (>150 kDa) no diffusion inside the PEM is found. To explore the influence of the polycations, films made with the branched Polyethylenimine (PEI) and PSS are investigated. These films show a strongly non-linear film growth and very broad internal interfaces. No interdiffusion occurs when these films are immersed in 1 M NaCl. To test the idea that PEI might serve as a diffusion barrier, a PEI layer is placed between a protonated and deuterated PDADMA/PSS block. Immersion of these multilayers in 1M NaCl solution for different times shows that the presence of PEI leads to a broadening of the interface which increases linearly with immersion time suggesting movement of PSS with constant slow speed.

CPP 9.27 Mon 17:30 Poster C

Influence of polymer molecular weight on the parabolic and linear growth of PDADMAC/PSS multilayers — ●PETER NESTLER and CHRISTIANE A. HELM — Inst. für Physik, Uni Greifswald, D-17487 Greifswald

The buildup of polyelectrolyte multilayers (PEMs) is investigated under in-situ conditions using multiple angle null ellipsometry. Polyanion PSS and polycation PDADMAC are adsorbed from 0.1 M NaCl solution. First the PEMs grow parabolically with the number of deposited layer pairs. This behaviour is attributed solely to the PDADMAC adsorption, while each PSS adsorption step leads to a constant thickness increase. After N_{trans} layer pairs a sharp transition from a parabolic to a linear growth occurs. Depending on the molecular weight of the polyelectrolytes, three different regimes of N_{trans} are found: For PDADMAC polymer weight above 100 kDa and PSS polymer weight above 30 kDa, the transition occurs constantly after 15 adsorbed layer pairs. In the case of lower molecular weights both polyelectrolytes show an opposite influence on N_{trans} . A lower PDADMAC polymer weight leads to a decrease (down to 8 layer pairs), and a lower PSS polymer weight to an increase of N_{trans} (up to 36 layer pairs), respectively. Interestingly, for each combination of molecular weight the value N_{trans} is roughly proportional to the thickness increase per deposited layer pair in the linear growth mode (between 4 nm and 23 nm).

CPP 9.28 Mon 17:30 Poster C

NREX polarized neutron/x-ray contrast reflectometer — ●OLAF SOLTWEDEL, YURY N. KHAYDUKOV, THOMAS KELLER, FRANZ TRALMER, MANFRED OHL, and BERNHARD KEIMER — Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

NREX is a classical angle dispersive, fixed wavelength neutron reflectometer at the cold neutron source of the FRM II in Garching/Munich. The instrument provides grazing incidence small angle scattering (GISANS), specular and off-specular reflectometry all in polarized and nonpolarized modes. These techniques are well suited to determine structural properties such as chemical aggregation, polymer and surfactant adsorption, interdigitation in low dimensions (surfaces, interfaces and thin film systems) at solid/liquid and solid/air interfaces. With a conventional x-ray add on ($CuK\alpha$), the instrument offers the unique possibility to combine x-ray- and neutron reflectometry in-situ. Recent developments, exemplary measurements and future

perspectives of NREX will be presented.

CPP 9.29 Mon 17:30 Poster C

Hindered Domain Formation of Lipid Monolayers with Adsorbed Macromolecules — •THOMAS ORTMANN, HEIKO AHRENS, and CHRISTIANE A. HELM — Inst. für Physik, Uni Greifswald, D-17487 Greifswald

Polyelectrolytes adsorb onto oppositely charged lipid monolayers either in a flatly disordered or a two-dimensional lamellar phase as known from Grazing Incidence Diffraction. With a Brewster angle microscope, nucleation and growth of lipid domains in the condensed phase are observed with short polyelectrolytes. These polyelectrolytes adsorb in a disordered phase when the lipids are in the fluid phase but order in the two-dimensional lamellar phase when the lipids are in the condensed phase. Long polyelectrolytes adsorb always in the two-dimensional lamellar phase beneath both lipid phases. Then, domain nucleation and growth is never observed. We suggest that the lipid rearrangement occurring on domain formation is not possible when to many lipids are electrostatically bound to one macromolecule.

CPP 9.30 Mon 17:30 Poster C

Imaging chemically patterned self-assembled monolayers with helium-ion microscopy — •DANIEL EMMRICH, HENNING VIEKER, ANDRÉ BEYER, and ARMIN GÖLZHÄUSER — Physics of Supramolecular Systems, University of Bielefeld, 33615 Bielefeld, Germany

Chemical patterning of certain self-assembled monolayers (SAMs) is possible by local exposure with electrons. In this way, for example, nitro groups of SAMs of NBPT (4'-nitro-1,1'-biphenyl-4-thiol) molecules convert into amino groups. This is accompanied by the formation of cross-links between molecules in the exposed monolayer. In this contribution the capability of helium-ion microscopy (HIM) for imaging chemical patterns in SAMs is discussed. To this end, SAMs of NBPT and BPT (1,1'-biphenyl-4-thiol) molecules are locally exposed by employing a stencil mask and an electron flood gun. HIM images of these samples at identical settings show a significant drop in the secondary-electron signal for the nitro-terminated areas in comparison to all other monolayer regions in this set of samples, i.e. the amino-terminated areas, the exposed as well as pristine SAMs from BPT molecules. This behaviour can be understood by considering the scattering of secondary electrons in the monolayer during the HIM imaging process. Imaging of fully cross-linked and chemically patterned SAMs as well as electron exposure dose sample series will be presented as well.

CPP 9.31 Mon 17:30 Poster C

Brushes of weak Polyelectrolytes (PE): Complex interactions with Solvent and Gold Nanoparticles — •ZULEYHA YENICE¹, JAN GENZER², RALF KÖHLER^{1,3}, and REGINE V. KLITZING¹ — ¹Stranski Lab, Inst. of Chemistry, TU Berlin, Germany — ²Dept. of Chemical & Biomolecular Engineering, NCSU, Raleigh, USA — ³Inst. of Soft Matter and Functional Materials, HZB, Berlin, Germany

PE-brushes represent a new class of thin film materials with tunable surface parameters and interactions, allowing functionalisation, or incorporation and exchange of solvents or particles. The swelling behaviour of PDMAEMA-brushes* was investigated by means of different solvents as ethanol and water of varying pH, and different water vapours. This ellipsometric study revealed a complex picture of the internal interactions of PE-brushes. Neutron reflectometry (NR) was used to determine, first, the structure of these films, either collapsed in dry state, or fully extended when swollen in buffer, secondly, the distribution and penetration depth of gold nanoparticles (Au-NP) in these brushes, after the exposure to suspensions of Au-NP with ca 5 or 15nm diameter. The study showed a comparatively homogeneous distribution of the brush length for our preparation technique. It proved that nanoparticles were incorporated into the PE-brushes irrespective from the size of the Au-NP and the length of the brush. But due to the complexity of the system it was not possible to determine a profile or horizon of deposition for the gold particles up to now. PE-brushes open a wide field for applications, and manifold of interesting, fundamental questions as well. *poly[2-(dimethylamino) ethyl methacrylate]

CPP 9.32 Mon 17:30 Poster C

Diffusion and demixing dynamics of water and ethanol in a self-adjusting molecularly thin slit-pore — •NIKOLAI SEVERIN, IGOR M. SOKOLOV, and JÜRGEN P. RABE — Department of Physics,

Humboldt-Universität zu Berlin Newtonstr. 15, 12489 Berlin, Germany

The behaviour of multicomponent liquids in confining geometries is a fundamental physical problem, which plays a central role in fields such as nano-fluidics, molecular biophysics, single molecule spectroscopy, and nano-chemistry, e.g. for molecular transport through channels of biological membranes, analyte recognition in molecular assays, and molecular synthesis. We followed with nanometer-scale lateral resolution the in-situ dynamics within mixed monomolecular water-ethanol films in a slit pore between mica and graphene, employing scanning force microscopy to image the graphene topography conforming to the film. Water and ethanol, highly miscible in three dimensions are shown to nano-phase separate in monolayers within the pore, consisting of a hydrophilic atomically flat mica surface and a more hydrophobic graphene layer. Graphene conforms to the liquid film, bending at the boundaries between the domains of water and ethanol to accommodate their different thicknesses of 80 ± 20 pm. The growth dynamics of the domains allows to determine a lower bound for the two-dimensional diffusion constant of ethanol in water of $D \geq 2 \times 10^{-14} \text{ ms}^{-2}$.

CPP 9.33 Mon 17:30 Poster C

Untersuchungen zur Bildung von Membranen auf Basis von Cellulosederivaten — •MICHAEL METZE¹, ANNETTE REICHE², STEPHAN BARBE² und DIETER MELZNER² — ¹Institut für Technische Chemie, Leibniz Universität Hannover, Deutschland — ²Sartorius Ste-dim Biotech GmbH, Göttingen, Deutschland

Poröse Polymermembranen auf Basis von Cellulosederivaten werden industriell häufig durch das Verdunstungsverfahren hergestellt. Dabei durchläuft ein Gießlösungsfilmen eine Phasenseparation, welche durch kontrollierten Entzug von Lösungsmitteln ausgelöst wird und bei weiterer Trocknung zur Bildung poröser Strukturen führt.

Das Verfahren wird großtechnisch zur Herstellung von Celluloseacetat- und Cellulosenitratmembranen mit Porengrößen im Bereich von $0,1 \cdot 10^3 \text{ m}$ eingesetzt, welche z. B. Grundlage von Filterprodukten und diagnostischen Produkten für die Biotechnologie sind.

Grenzflächeneffekte sollten eine entscheidende Rolle bei der Membranbildung spielen. Allerdings ist ihr Beitrag nicht bekannt da die Energiebilanz des Verfahrens durch die Verdunstung der Lösungsmittel dominiert wird und die Flory-Huggins Thermodynamik zur Beschreibung der Polymerlösung keinen Ansatz zur Berücksichtigung von Grenzflächenphänomenen bietet.

Die Erfahrung zeigt, dass Tenside Einfluss auf den Membranherstellungsprozess haben. Im Rahmen des Vortrags soll, ausgehend von einem quaternären Modellsystem mit bekanntem Phasendiagramm, der Einfluss verschiedener Tenside auf das Entmischungsverhalten der Gießlösung durch Trübungstitration, gezeigt werden.

CPP 9.34 Mon 17:30 Poster C

Hydrodynamic description of free surface films of nematic liquid crystals: weak anchoring model — •TE-SHENG LIN and UWE THIELE — Department of Mathematical Sciences, Loughborough University, Loughborough, Leicestershire LE11 3TU, UK

We propose a long-wave model that describes the dynamics of a free surface thin film of nematic liquid crystals on a solid substrate under weak anchoring conditions at the free surface. The model recovers two regimes reported in the literatures: (i) For thick films the surface anchoring energy dominates. The molecules in the bulk have to bend across the film (HAN state) and lead to strong 'elastic diffusion' of the free surface height; (ii) For thin films the bulk elastic energy dominates. The orientation of the molecules is homogeneous in the bulk (P state) and has no influence on the stability of the free surface. Furthermore, it is found that there exists an intermediate film thickness range for which the free surface is linearly unstable. Finally, we show that the P state, even though neutrally stable, is actually nonlinearly unstable.

CPP 9.35 Mon 17:30 Poster C

Morphology of ultrathin gallium oxide layers — •FRANK LAWRENZ¹, NIKOLAI SEVERIN², JÜRGEN P. RABE², CHRISTIANE A. HELM¹, and STEPHAN BLOCK³ — ¹Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Str. 6, D-17487 Greifswald, Germany — ²Department of Physics, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — ³ZIK HIKE, Fleischmannstr. 42 - 44, D-17475 Greifswald, Germany

Liquid gallium is applied onto mica, silicon and silica surfaces. AFM tapping mode imaging shows micrometer sized gallium drops accompanied by extended, ultrathin layers, which we attribute to gallium

oxide (GaOx) films passivating the surface of liquid gallium under ambient conditions. On all surfaces investigated, the GaOx layers exhibit a thickness of about 3 nm and a roughness similar to the underlying substrate. Although they replicate patterns of the substrate topography, they also exhibit high mechanical stability, as normal forces on the order of 1 μN (for tip radii of some 10 nm) have to be applied to abrade the layer. We discuss different methods of liquid gallium application onto the surfaces which lead to ultrathin GaOx layers of different quality with respect to layer homogeneity and coated area.

CPP 9.36 Mon 17:30 Poster C

Asymptotics of the Capillary-Driven Thin Film Equation — •THOMAS SALEZ¹, MICHAEL BENZAQUEN¹, JOSHUA D. MCGRAW², OLIVER BÄUMCHEN², KARI DALNOKI-VERESS², and ELIE RAPHAËL¹ — ¹Gulliver, ESPCI, Paris, France — ²McMaster University, Hamilton, Canada

The study of polymer nanofilms is of tremendous importance in a variety of scientific fields, such as polymer physics, physiology, biophysics, micro-electronics, surface chemistry, and applied mathematics. In the lubrication approximation for viscous flows, the evolution of the free surface of such a film is governed by the capillary-driven thin film equation. We hereby present analytical [1] and numerical [2] treatments of this partial differential equation for a stepped initial profile, and compare the results to experiments on polystyrene [3]. Then, we derive the Green's function of the linearized problem and therefore obtain the solution for any summable initial perturbation. In particular, we show that this solution uniformly converges in time towards a unique self-similar attractor that is precisely the Green's function multiplied by the algebraic volume of the perturbation [4]. Finally, a numerical scheme enables us to conjecture the extension of this result to the non-linear case, where the universal attractor appears to be identical to the one obtained in the linear case.

[1] Salez et. al PoF 24 102111 (2012), [2] Salez et al. EPJE 35 114 (2012), [3] McGraw et al. PRL 109 128303 (2012), [4] Benzaquen et al. submitted to SIAM (2012)

CPP 9.37 Mon 17:30 Poster C

Growth kinetics of metal films sputtered on adhesive polymer films followed with in-situ GISAXS — •MARKUS SCHINDLER¹, EZZELDIN METWALLI¹, GÖKHAN GÜMÜSSOY¹, PETER MÜLLER-BUSCHBAUM¹, and STEPHAN V. ROTH² — ¹TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany — ²HASYLAB at DESY, 22603 Hamburg, Germany

Pressure sensitive adhesives (PSAs) are widely used in everyday applications, industries and medicine. Individually tailored compounds exist for many fields of application. Among these is the establishment of strong but reversible adhesive bonds between metal surfaces. The interactions between a metal adherent and the polymeric adhesive govern the performance of any metal-adhesive joint and are therefore important to understand. We present an in-situ grazing incidence small angle X-ray scattering (GISAXS) study on the growth of metal films sputtered on a model PSA as well as on its homopolymer components. Different growth kinetics reveal insights into the metal-polymer interactions and isolate the influence of atomic and molecular forces due to the absence of usual adherent surface properties like its roughness or preceding surface treatments, e.g. cleaning. GISAXS provides means to follow the metal film formation during sputtering in-situ, revealing structural information with a very high time resolution.

CPP 9.38 Mon 17:30 Poster C

Non-equilibrium dynamics of a bilayer system of confined colloidal particles in a planar shear flow — •TARLAN A. VEZIROV and SABINE H. L. KLAPP — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

We perform computer simulations of a confined bilayer system of charged colloidal particles interacting via a combined soft-sphere- and Yukawa-potential. The system is driven from equilibrium by a planar shear flow. The model parameters are adjusted according to ludox silica particles, which we have previously studied under equilibrium conditions [1,2]. As a framework for solving the equation of motion, we employ overdamped Brownian dynamics simulations. We investigate the impact of the shear flow and confinement on structure formation and focus on statistical properties such as e.g. translational symmetry orderparameter and pair distribution functions. Furthermore we are interested in the emergence of the zigzag motion observed in experiments [3] and characterized by the spatial oscillations of layers. We

hope that our results can be used as predictions for future experimental work.

[1] S. Grandner and S.H.L. Klapp, J. Chem. Phys. **129**, 244703 (2008). [2] S. H. L. Klapp, Y. Zeng, D. Qu and R. v. Klitzing, Phys. Rev. Lett. **100**, 118303 (2008). [3] D. Derks, Y.L. Wu, A.v. Blaaderen and A. Imhof, Soft Matter **5**, 1060 (2009).

CPP 9.39 Mon 17:30 Poster C

Effect of patterning on film morphology and device performance of BHJ organic solar cells — •DANIEL MOSEGUÍ GONZÁLEZ¹, CLAUDIA M. PALUMBINY¹, JAN PERLICH², STEPHAN V. ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department E13, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85747 Garching (Germany) — ²HASYLAB at DESY, Notkestr. 85, 22603 Hamburg (Germany)

Controlling morphology within polymer films for solar cells through imprinting procedures has been found to be a promising pathway to achieve high efficiency devices. These structured devices are expected to present improved performance due to light scattering and reflection effects, which lead to enhanced absorption without increasing film thickness. Furthermore, in the case of poly(3-hexylthiophene) a change in the crystalline orientation was observed, leading to higher conductivities and better device performance. So far limited work has been carried out investigating the inner morphological changes of imprinted blend devices. In this work, the effects of structuring BHJ poly(3-hexylthiophene): phenyl-C61-butyric acid methyl ester (P3HT:PC60BM) films are investigated. Imprinted surfaces are characterized with AFM. Moreover, crystallinity and internal film morphology is characterized using grazing incidence wide/small angle x-ray scattering (GIWAXS/GISAXS), respectively. In addition, x-ray reflectivity measurements provide supporting information for depth profiles. Finally, the characteristics of the device performance will be discussed and compared to the observed morphological changes.

CPP 9.40 Mon 17:30 Poster C

Nanostructured Organic Solar Cells — •THOMAS PFADLER, RICKY DUNBAR, and LUKAS SCHMIDT-MENDE — Dept. of Physics, University of Konstanz, 78457 Konstanz, Germany

Organic solar cells have the potential to become an important low-cost alternative to conventional solar cells. However, before this can happen, the energy harvesting potential of organic solar cells must become more comparable with that of the pervading technology. This research is focusing on nanoimprint lithography (NIL), a low-cost lithographic method for high-throughput patterning applicable to organic semiconductors. This technique can be used to tailor an organic solar cells active material on a nanometer scale.

One possible application is the implementation of a plasmonic light-trapping geometry by structuring the organic semiconductor metal interface e.g. the back-electrode of a bulk heterojunction device. Another promising application of NIL aims to control the nanostructure of a donor-acceptor interface in organic devices. One organic layer e.g. the hole accepting layer is structured before the electron acceptor is subsequently deposited. Target of this approach is to enhance the overall efficiency by enhancing the interfacial area increasing the exciton separation yield and ensuring direct pathways to the electrodes minimizing charge recombination.

CPP 9.41 Mon 17:30 Poster C

Coat Thickness Dependent Adsorption of Hydrophobic Molecules at Polymer Brushes — •JENS SMIATEK¹, HENDRIK WAGNER², CARSTEN HENTSCHEL³, LIFENG CHI³, ARMIDO STUDER², and ANDREAS HEUER⁴ — ¹Institut für Computerphysik, Universität Stuttgart, Germany — ²Institut für Organische Chemie, WWU Münster, Germany — ³Physikalisches Institut, WWU Münster, Germany — ⁴Institut für Physikalische Chemie, WWU Münster, Germany

We study the adsorption properties of hydrophobic test particles at polymer brushes with different coat thicknesses via mesoscopic Dissipative Particle Dynamics simulations. Our findings indicate stronger adsorption energies at thin polymer brushes. The reason for this difference is mainly given by entropic contributions due to different elastic deformations of the coatings. The numerical findings are supported by analytical calculations and are in good agreement to experimental fluorescence intensity results.

CPP 9.42 Mon 17:30 Poster C

Distribution of Gold Nanoparticles within patterns of Polymer Brushes using UV lithography — •STEPHANIE CHRISTAU,

JIANLI ZHAO, and REGINE VON KLITZING — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Institute for Chemistry, Technical University Berlin, Straße des 17. Juni 124, 10623 Berlin, Germany

The distribution of Gold Nanoparticles (AuNPs) in polymer brushes which are grafted from planar silicon surfaces is of big interest in the last few years. The reason is that polymer brushes are promising candidates for the ordering of particles and AuNPs will induce interesting optical properties.

Polymer brushes of (N,N-dimethylamino)ethyl methacrylate (DMAEMA) and N-isopropylacrylamide (NIPAM) are grown from

a 2-bromo-2-methyl-(3-(triethoxysilyl)propyl)propanamide (BTPAm)-covered silicon surface via surface-initiated atom transfer radical polymerization (SI-ATRP). For the synthesis of both initiator-covered self-assembled monolayer (SAM) and polymer brushes a new type of sealed reactor is used that provides a constant nitrogen flux. The grafted chains are investigated using ellipsometry, atomic force microscopy (AFM), X-ray reflectometry, scanning electron microscopy (SEM) and gel permeation chromatography (GPC).

To study the influence of the polymer's chemical composition, the brush thicknesses and the conformation on the particle distribution, grid-like patterns of polymer brushes are formed using UV lithography. Different approaches for patterning are addressed.

CPP 10: Poster: Charge transfer effects in molecular materials (related to symposium SYCT)

Time: Monday 17:30–19:30

Location: Poster C

CPP 10.1 Mon 17:30 Poster C

Foam-like structures of titania films for application in flexible photovoltaic — ●BO SU, MARTIN A. NIEDERMEIER, MONIKA RAWOLLE, and PETER MÜLLER-BUSCHBAUM — TU München, Physik Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany

Due to high surface to volume ratio and their bicontinuous morphology, foam-like nanostructures are becoming more interesting in photovoltaics, for example in hybrid solar cells and dye-sensitized solar cells (DSSC). The nanoporous titania layers are responsible for the electron transporting and directing dye layers' structure. In our studies, the morphology of titania films is investigated with respect to a possible incorporation into hybrid solar cells. The titania films are prepared by a sol-gel process in combination with block copolymer templating. Via this route we have a very high level of control over the final morphology. The films are typically prepared via spin-coating, followed by a calcination step to remove the polymer template and obtain crystalline titania. Additionally, our method is even suitable for low-temperature synthesis by changing the titania precursor. The structure of these films is probed with the imaging techniques such as scanning electron microscopy and atomic force microscopy. To determine the optical and opto-electronical properties UV/Vis spectroscopy and photoluminescence are used.

CPP 10.2 Mon 17:30 Poster C

Field dependent charge carrier generation via charge transfer states: A blending ratio dependent study — ●JULIA KERN¹, CLEMENS GRÜNEWALD¹, HANNES KRAUS¹, FRANZISKA FUCHS¹, CARSTEN DEIBEL¹, and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius Maximilians University of Würzburg, 97074 Würzburg, Germany — ²Bavarian Center for Applied Energy Research e.V. (ZAE Bayern), 97074 Würzburg, Germany

In organic bulk heterojunction solar cells, the mechanism of exciton dissociation at the polymer–fullerene interface is still controversially debated. This work studies the charge carrier generation via charge transfer states by investigating the electric field dependence of the process for a model system consisting of MDMO-PPV and PC₆₁BM. Focusing on the influence of different donor–acceptor blend ratios, the complementary techniques of field dependent photoluminescence quenching and transient absorption are employed to reveal a substantial change in the electric field behavior. Thus, the binding energy of the respective charge transfer excitons (CTE) is reduced from ~ 320 meV for a 4:1 blend ratio to ~ 200 meV for a 1:1 blend, decreasing even further for higher PC₆₁BM concentrations. The observed phenomenon may be ascribed to a change in the average dielectric constant or in the CTE delocalization length of the system. The relevance of these influencing factors is unveiled by combined morphological studies comprising atomic force microscopy and optically detected magnetic resonance. This study demonstrates the importance of a high dielectric constant for charge carrier generation in organic photovoltaics.

CPP 10.3 Mon 17:30 Poster C

Effect of Polymorphism, Regioregularity and Paracrystallinity on Charge Transport in Poly(3-Hexyl-Thiophene) [P3HT] Nanofibers — ●CARL POELKING, KURT KREMER, and DENIS ANDRIENKO — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

We establish the link between molecular order and charge-transport parameters in poly(3-hexyl-thiophene) (P3HT) accounting for different polymorphic structures and regioregularities. Using atomistic molecular dynamics, we study structural transitions related to side-chain melting and a conversion from a non-interdigitated metastable (form I') to the stable (form I) P3HT polymorph, as also observed experimentally, thus providing structural models for side-chain arrangement and backbone-backbone stacking. We investigate how packing modes and regioregularity effect paracrystalline and side-chain order and analyse effects thereof on the dynamics and distribution of electronic couplings and site energies. In particular, we demonstrate how a small concentration of defects in side-chain attachment can lead to a dramatic decrease in charge-carrier mobility due to a strong intermolecular contribution to the energetic disorder, which we attribute to fluctuations in backbone-backbone distances. Our simulated mobilities indicate excellent agreement with experimental values obtained for P3HT nanofibers.

CPP 10.4 Mon 17:30 Poster C

Microscopic simulations of charge and energy transfer in crystalline PCPDTBT and PSBTBT — ●ANTON MELNYK, BJÖRN BAUMEIER, and DENIS ANDRIENKO — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Charge and exciton transfer processes in two semi-crystalline polymers, PCPDTBT and PSBTBT, are compared using a combination of classical molecular dynamics to simulate semi-crystalline morphologies, quantum chemistry to evaluate the electronic structure of conjugated segments, and charge/energy transfer theories to study charge and energy transfer/transport. By linking local molecular arrangements of two polymers to the changes in distributions of site energies and electronic coupling elements we rationalize the improved charge mobility, reduced bimolecular recombination, and formation of charge transfer states in PSBTBT.

CPP 10.5 Mon 17:30 Poster C

Multifrequency electron spin resonance analysis of organic polymer:fullerene blends — ●MAX GESSNER¹, ANDREAS SPERLICH¹, HANNES KRAUS¹, STEFAN VÁTH¹, and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius Maximilian University Würzburg, 97074 Würzburg, Germany — ²ZAE Bayern, 97074 Würzburg, Germany

Understanding of the light-induced charge transfer in organic solar cells is essential to improve material properties and processing parameters, and, at long sight, device performance. Since the charge carriers are spin- $\frac{1}{2}$ particles they can be studied by electron paramagnetic resonance (EPR). Several solar cell blends of fullerene-derivatives PC₆₀BM and PC₇₀BM with conjugated polymers P3HT, C-PCPDTBT and Si-PCPDTBT were investigated with light induced X-band EPR. The resulting spectra consist of overlapping signals from electrons and holes. By performing the same measurements with the high frequency Q-band EPR we were able to study the individual signals of charges localized on either fullerene or polymer domains in more details with higher resolution. By comparing the experimental spectra with simulations performed with EasySpin we have the tool for learning more about the local order and geometry as well as the electric properties of these promising materials for organic photovoltaics.

CPP 10.6 Mon 17:30 Poster C

Influence of charge density on microscopic transport in amorphous organic semiconductors — ●PASCAL KORDT and DENIS ANDRIENKO — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

The effect of finite charge carrier density on microscopic transport parameters, such as occupation probabilities, local currents, and charge mobility is analyzed by means of the off-lattice kinetic Monte Carlo method as well as the Fokker-Planck equation in a mean-field approximation. Implications for the macroscopic description of organic field effect transistors and light emitting diodes are discussed.

CPP 10.7 Mon 17:30 Poster C

Energy Level Alignment for Many-Body Resonant Tunneling — ●JESSICA WALKENHORST¹, HEIKO APPEL², NICOLE HELBIG^{3,1}, and ANGEL RUBIO¹ — ¹NanoBio Group and ETSF, UPV/EHU, Spain — ²NanoBio Group and ETSF, Fritz-Haber-Institut der MPG, Germany — ³PGI and IAS, Forschungszentrum Jülich, Germany

Electron tunneling plays a fundamental role in many chemical and physical processes and provides evidence of quantum mechanics at the macroscopic level. In addition to the fundamental physics, electron tunneling at surfaces also attracts much attention due to its importance for charge transfer and carrier injection mechanisms e.g. in organic devices. Resonant tunneling is governed by the alignment of energy levels of donor and acceptor. While the separate systems are described well by standard approaches, the alignment of their chemical potentials is problematic since bringing donor and acceptor in contact changes the respective energy levels due to the electronic interaction. We investigate resonant many-body tunneling in a one dimensional donor-acceptor system, where the electrons interact via a softened Coulomb potential. For a system of few electrons, we solve the Schrödinger equa-

tion exactly. As a first step we analyze the case of adiabatic tunneling. Starting from the description of tunneling between non-interacting systems, we derive the necessary energy correction terms for the case of the complete fully interacting donor-acceptor many-body system. We then extend our adiabatic model to a time-dependent description to study the deviation of the dynamic tunneling behavior from the adiabatic case.

CPP 10.8 Mon 17:30 Poster C

Microscopic simulations of electronic excitations at donor-acceptor interfaces — ●BJÖRN BAUMEIER, CARL POELKING, and DENIS ANDRIENKO — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Fundamental processes involving electronic excitations govern the functionality of molecular materials, in which the motion of excitons and charges is determined by an interplay of molecular electronic structure and morphological order. To understand, e.g., charge separation and recombination at donor-acceptor heterojunctions in organic solar cells, knowledge about the microscopic details influencing these dynamics in the bulk and across the interface is required.

Using a combination of molecular dynamics and quantum-chemistry (DFT/GW-BSE), we first obtain atomistically resolved morphologies of prototypical planar heterojunctions of dicyanovinyl-substituted quaterthiophene (donor) and C₆₀ (acceptor) and then analyze the charged and neutral electronic excitations therein. We pay special attention the spatially-resolved electron/hole transport levels (band bending and offsets), as well as the relative energies of Frenkel and charge-transfer excitations at the interface. Finally, we link our results to the molecular architecture of the donor material and its orientation on the fullerene substrate.

CPP 11: Poster: Glasses and Glass Transition (joint session DY/CPP)

Time: Monday 17:30–19:30

Location: Poster C

CPP 11.1 Mon 17:30 Poster C

Room temperature ionic liquid's (RTILs) dynamic glass transition by calorimetric methods. — ●EVGENI SHOIFET^{1,2}, HEIKO HUTH¹, SERGEY VEREVKIN², and CHRISTOPH SCHICK¹ — ¹Institute of Physics, Rostock University, Rostock, 18051, Germany — ²Institute of Chemistry, University of Rostock, 18051 Rostock, Germany

Many of the ionic liquids are good glass formers. Nevertheless, only a few studies of the glass transition in ionic liquids are available so far. Particularly the frequency dependence of the dynamic glass transition (α -relaxation) is not known for most ionic liquids. The standard technique for such studies - dielectric spectroscopy - is not easily applicable to ionic liquids because of the high electrical conductivity. We try to use calorimetric techniques to obtain complex heat capacity and to investigate the dynamic glass transition of room temperature ionic liquids (RTILs) in a wide frequency range. This can give an insight in cooperative motions of ions and ion clusters in RTILs. The techniques that were used are DSC, TMDSC, and AC-chip calorimeter^[5] covering a frequency range from 0.001 Hz to 10000 Hz. Similar fragility was found not only in series of RTILs with different alkyl chain length in the cation ([C_nmim]), but also for two different anions ([Co(NCS)₂], [NTf₂]). Also the decrease in thermal glass transition temperature (T_g) and add/even effect have been observed in cobalt RTIL, while the T_g in RTIL with sulfonic anion is increasing, with increase of alkyl chain length.

CPP 11.2 Mon 17:30 Poster C

Nanoscale confinement of a low molecular weight liquid — ●ANNA DJEMOUR, JÖRG BALLER, CARLO DI GIAMBATTISTA, MARLENA FILIMON, JENS-PETER BICK, ANDREAS MICHELS, and ROLAND SANCTUARY — Laboratory for the Physics of Advanced Materials, University of Luxembourg, 162A, Avenue de la Faiencerie, L-1511 Luxembourg

The enormous change of the molecular dynamics of glass formers when approaching the thermal glass transition temperature is usually attributed to the increase of the size of cooperative rearranging regions (CRR). Spatial confinement is known to take influence on the glass transition behaviour when the scale of confinement is in the same order as the size of the CRRs. In this work we present investigations of the glass transition of a low molecular weight epoxy resin (Diglycidil

Ether of Bisphenol A, DGEBA) filled in different nanoporous silica glasses. The effect of confinement is studied by two different ways: i) properties of the glass former are investigated by modulated calorimetry, dielectric spectroscopy and X-ray scattering. ii) properties of the whole system, i.e. porous glasses filled with the glass former are investigated by thermo-mechanical analysis and dynamic mechanical analysis. Combining the results from both approaches contributes to the understanding of the glass former DGEBA under confinement.

CPP 11.3 Mon 17:30 Poster C

Local Thermal Analysis as a Tool for Morphological Investigation of Polypropylene — THOMAS FISCHINGER, ●LISA MARIA UBERLACKER, and SABINE HILD — Institute for Polymer Science, Johannes Kepler University, Altenbergerstraße 69, 4040 Linz, Austria

A basic understanding of physical and chemical properties of polymers is of fundamental importance for the development of advanced polymers. Thermal analysis methods are generally used to provide important and reliable data. However, up to now mainly bulk properties of polymers have been detected. Conventional methods reach a limit for applications such as the investigation of crystal structures. Therefore, a method is proposed for nano-thermal characterization of polymers using scanning probe microscopy (SPM) in combination with heatable cantilever probes. This method is based on an appropriate temperature calibration, which provides a reliable correlation between applied voltage and the temperature at the tip. LTA measurements were applied to high molecular isotactic polypropylene with varying lamellar thicknesses. Furthermore, the structure and morphology of randomly distributed isotactic propylene-1-hexene-copolymer (PHCP) were investigated with a focus on local thermal properties. In this study it will be shown that it is possible to investigate the differences in softening of α - and γ - structure of PHCP.

CPP 11.4 Mon 17:30 Poster C

Bestimmung der molekularen Dynamik von Polyvinylpyrrolidon mittels NMR und DS — ●MICHAEL LANNERT und MICHAEL VOGEL — Technische Universität Darmstadt, Institut für Festkörperphysik

Die molekulare Dynamik von Wasser in Polymer-Matrizen (D₂O-Polyvinylpyrrolidon-Mischung) wurde mittels Deuteronen NMR un-

tersucht. Fragestellung ist, ob sich anhand der temperaturabhängigen Korrelationszeit der Rotation der C-D-Bindungen ein starkes oder fragiles Verhalten ausmachen lässt. Eine Theorie, welche die Existenz einer hochdichten (HDL) und niederdichten (LDL) Flüssigphase des Wassers im unterkühlten Regime voraussagt, legt einen "Fragil-Stark-Übergang" bei $T \approx 220\text{K}$ nahe. Zusätzlich zu den NMR-Messungen wurden Daten aus Dielektrischer Spektroskopie ausgewertet. Unter Annahme spezieller empirischer Modelle für die spektrale Dichte der unterliegenden Prozesse, namentlich einer Cole-Davidson Verteilung, kann so aus den DS Daten die mittlere Relaxationsrate der NMR-Experimente vorausgesagt und mit den tatsächlich erhaltenen Werten verglichen werden. Interpolationen der Temperaturabhängigkeit der Wasserdynamik mit einem Arrheniusgesetz ergeben eine Aktivierungsenergie von $E_A = 0.5\text{eV}$, welche von der Wasserkonzentration unabhängig ist. Durch Kombination von NMR und DS sowie Abdeckung eines breiten Zeitfensters gelingt es somit, ein konsistentes Bild der Dynamik im untersuchten System zu zeichnen.

CPP 11.5 Mon 17:30 Poster C

Thermomechanical Properties of Organic-Coatings: A scanning force microscopy study — ●BERNHARD JACHS¹, BERNHARD STRAUSS², and SABINE HILD¹ — ¹Institute of Polymer Science, JKU Linz, Altenbergstraße 69, 4040 Linz, — ²voestalpine Stahl GmbH, 4020 Linz

Coil Coating is a continuous industrial process where one or more polymeric layers with thicknesses ranging from 5 up to 50 μm are applied on steel coils to protect them against environmental impacts. For further processing of the coated material, the knowledge of thermal and mechanical properties of the coating is crucial. Widely used analytical techniques (DSC, DMA) require special sample preparation where the coating has to be removed from the substrate or is prepared as a free standing coating film. In this work a SFM equipped with a heating stage was used to directly investigate mechanical properties of coatings as a function of temperature by performing nanoindentation measurements. Static measurements were carried out at different displacement rates and temperatures. By taking into account contact-mechanical models, which describe the tip-sample-interaction, the Elastic Modulus can be obtained as a function of temperature and displacement rate. Shifting the curves according to the Williams-Landel-Ferry equation yields a mastercurve which allows extrapolating mechanical properties beyond the measuring range. In addition, dynamic measurements have been carried out modulating the tip position at different frequencies and temperatures. Using proper viscoelastic models, Storage and Loss Moduli as well as loss tangent can be determined.

CPP 11.6 Mon 17:30 Poster C

In-situ investigation of vapor-deposited thin films of toluene and ethylbenzene by AC chip-nanocalorimetry — ●MATHIAS AHRENBERG¹, KATIE R. WHITAKER², YEONG-ZEN CHUA¹, HEIKO HUTH¹, MARK D. EDIGER², and CHRISTOPH SCHICK¹ — ¹Institut für Physik, Universität Rostock, Wismarsche Str. 43-45, 18051 Rostock, Germany — ²Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA

Physical vapor deposition can be used to produce thin films with particular material properties. For example extraordinarily stable glasses can be obtained from organic molecules like toluene and ethylbenzene. We have investigated properties like packing efficiency and kinetic stability depending on substrate temperature and deposition rate by in-situ AC chip-nanocalorimetry. We have varied the substrate temperature covering the range from temperatures proven to yield high enthalpy glasses up to temperatures proven to yield low enthalpy glasses. This way the complete evolution of the mentioned stable glass properties is observed. Moreover AC calorimetry offers the possibility for isothermal measurements which enables to follow the transformation of the stable glass to the super-cooled liquid. Transformation experiments give suggestion of the transformation mechanism and its temperature dependence. The data are in agreement with a growth front for the transformation of the stable glass into the supercooled liquid.

CPP 11.7 Mon 17:30 Poster C

Triplet-Solvatationsdynamik an unterkühlten Wassermischungen in hartem und weichem Confinement — ●VINCENTO TALLUTO¹, CARL BÖHMER¹, THOMAS WALTHER¹ und THOMAS BLOCHOWICZ² — ¹Institut für Angewandte Physik, Technische Universität Darmstadt, Schlossgartenstr. 7, 64289 Darmstadt — ²Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstraße 8, 64289 Darmstadt

Die Triplet-Solvatationsdynamik ist eine Methode, mit der Relaxation in unterkühlten Flüssigkeiten nahe des Glasübergangs untersucht werden kann. Hierzu wird der Flüssigkeit ein Farbstoff beigemischt, welcher mittels eines UV-Laserpulses in einen langlebigen Tripletzustand angeregt wird. Über den zeitlichen Verlauf der Emissionswellenlänge des Farbstoffes kann die Relaxation der Solvatationshülle in einem Zeitbereich von 0.1 ms bis 1 s verfolgt werden. Je nach Farbstoff kann dabei eine dielektrische oder mechanische Response auf die Anregung des Farbstoffmoleküls beobachtet werden.

Der Vorteil dieser lokalen Methode liegt u.a. darin, dass z. B. Glasbildner in Confinement untersucht werden können. In gefüllten Porensystemen sind hier z. B. die Ergebnisse der herkömmlichen dielektrischen Spektroskopie nur schwer zu interpretieren. Wir präsentieren erste Messungen an Wasser-Alkohol-Mischungen als Bulk-Material, sowie im Confinement von Vycor-Poren und Mikroemulsionströpfchen mit dem Ziel, Oberflächen-, Dichte- und Finite-Size-Effekte voneinander zu trennen, deren Überlagerung eine eindeutige Interpretation dynamischer Daten bisher erschwert.

CPP 11.8 Mon 17:30 Poster C

The interplay between inter- and intramolecular dynamics in a series of alkylcitrate — ●WYCLIFFE KIPNUSU¹, WILHELM KOSSACK¹, CIPRIAN IACOB¹, JOSHUA SANGORO², and FRIEDRICH KREMER¹ — ¹Institute of Experimental Physics I, University of Leipzig, Linnestr. 5, 04103 Leipzig, Germany — ²Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830-6197, United States.

The inter- and intra-molecular dynamics in a series of glass-forming alkylcitrate is studied by a combination of Broadband Dielectric (BDS), Pulsed Field Gradient Nuclear Magnetic Resonance (PFG NMR), Dynamic Mechanical (DMS), and Fourier-Transform Infrared (FTIR) Spectroscopy. Analyzing the temperature dependencies of specific IR absorption bands in terms of their spectral position and the corresponding oscillator strengths enables one to unravel the intramolecular dynamics of specific molecular moieties and to compare it with the intermolecular dynamics. With decreasing temperature, the IR band positions of carbonyls and H-bonded moieties of citrates, show a red shift with a kink at T_g while other moieties whose dynamics are decoupled from those of the core units, exhibit a blue shift with nominal changes at T_g . The oscillator strength of the ester linkage and H-bonded units show a kink at a temperature where structural and faster secondary relaxations merge. By that, a wealth of novel information is obtained proving the fundamental importance of intramolecular mobility in the process of glass formation, beyond coarse-grained descriptions. Reference: Papadopoulos P. et al. *Softmatter* 2012 In press.

CPP 11.9 Mon 17:30 Poster C

First Thermal Conductivity and Elastic Susceptibility measurements of Zr-based Bulk Metallic Glasses at Ultra Low Temperatures — ●MARIUS HEMPEL, DANIEL ROTHFUSS, ANDREAS FLEISCHMANN, and CHRISTIAN ENSS — Kirchhoff-Institut für Physik, Heidelberg

The thermal conductivity and the elastic susceptibility of Zr-based superconducting bulk metallic glasses have been measured the first time in the temperature range down to 6 mK in order to study the interaction of atomic tunnelling systems with phonons and conducting electrons. Additional susceptibility measurements reveal a superconducting transition around 1 K.

Both, the elastic susceptibility and the thermal conductivity measurements use a novel SQUID-based contact free detection technique below 1 K which allows to dispense with a bias voltage in the case of the elastic measurements and reduces parasitic heat input during the thermal conductivity measurements.

The thermal conductivity of the bulk metallic glass $\text{Zr}_{52.5}\text{Ti}_5\text{Cu}_{17.9}\text{Ni}_{14.6}\text{Al}_{10}$ scales nearly quadratically with temperature as expected from the tunnelling model. The change of sound velocity of the of the bulk metallic glass $\text{Zr}_{55}\text{Cu}_{30}\text{Al}_{10}\text{Ni}_5$ shows a temperature dependence which is governed by resonant and relaxational processes. The latter are caused by the interaction with thermal phonons and quasi-particles in the vicinity of the superconducting transition.

CPP 11.10 Mon 17:30 Poster C

Non-universal dielectric and elastic properties of glasses at very low temperatures — ●ANNINA LUCK, MARIUS HEMPEL, ANDREAS FLEISCHMANN, and CHRISTIAN ENSS — Kirchhoff-Institut für Physik, Universität Heidelberg

Based on many experimental observations the low temperature properties of glasses, governed by atomic tunneling systems, have long been viewed as being universal. In the last years, however, measurements of dielectric two-pulse polarization echoes have revealed that nuclear electric quadrupole moments involved in atomic tunneling systems can cause large material-dependent effects in magnetic fields.

To study the possible influence of nuclear electric quadrupoles in two level systems on the low frequency dielectric and elastic properties of glasses down to a temperature of 10 mK, we measured vitreous silica and the multicomponent glass N-KZFS11, which contains 25 mass percent of tantalum oxide. As ^{181}Ta carries a very large nuclear electric quadrupole moment, N-KZFS11 seems to be an ideal candidate to determine the influence of nuclear electric quadrupole moments on the physical properties of glasses at low temperatures.

Our measurements not only show a non-universal dielectric and elastic behaviour for these two glasses, but the results also differ significantly from various predictions of the standard tunneling model. We discuss these new findings and possible implications in terms of the tunneling model.

CPP 11.11 Mon 17:30 Poster C

1/f flux noise induced by spin glasses in superconducting qubits — ●JUAN ATALAYA — Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie, Karlsruhe, Deutschland.

Recently, it has been realized that the coherence time of flux qubits is limited by unknown sources of flux noise, which exhibits a $1/f$ spectrum at low frequencies $f \lesssim 10\text{kHz}$ and at low temperatures $\lesssim 5\text{K}$. Experiments suggest that the main contribution to the flux noise may be produced by paramagnetic spins located on the surface of the superconducting loop. We consider a spin glass system of classical Heisenberg spins and investigate the low frequency dynamics of the total magnetization at temperatures near the spin glass freezing temperature. We discuss the role of anisotropy and temperature on the shape of the noise spectrum.

CPP 11.12 Mon 17:30 Poster C

Glassy dynamics of orientation fluctuations in modulated phases — ●CHRISTIAN RIESCH, GÜNTER RADONS, and ROBERT MAGERLE — Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz

We report on glassy dynamics and aging behavior in a 2D stripe-forming system free of topological defects. Numerical simulations based on model B with Coulomb interactions were performed for a wide range of noise strengths. The autocorrelation function of the local stripe orientation obeys the scaling form $C_\theta(t, t_w) \sim t_w^{-b} \cdot f(t/t_w)$, typical for glassy dynamics, and we argue that the relaxation time of the orientation fluctuations diverges. Spatial correlations are anisotropic, exhibiting a fast decay parallel to the stripes and an emerging power-law behavior in the perpendicular direction. We also investigate aging effects in other modulated phases, such as a hexagonal system in 2D and a lamellae-forming system in 3D.

CPP 11.13 Mon 17:30 Poster C

Theoretical methods to analyse scattering patterns in the systems of self-assembling anisotropic particles — ●SOFIA KANTOROVICH^{1,2}, ELENA PYANZINA¹, CRISTIANO DE MICHELE², and FRANCESCO SCIORTINO² — ¹Ural Federal University, Lenin av. 51, 620000, Ekaterinburg, Russia — ²Sapienza, University of Rome, Piazza A. Moro 5, 00185, Rome, Italy

Self-assembly is a phenomena which can be observed on the broad range of scales: starting from simple molecules to colloidal particles. This effect of spontaneous equilibrium formation of reversible aggregates might serve as a key to the synthesis of new smart materials, once self-assembly mechanisms are well understood. The aggregates

formed in the systems might lead to significant changes in macroscopic responses of the systems, thus, becoming very important in soft matter and biophysics. One of the examples of self-assembling building blocks is short blunt-ended DNA duplexes which form chains. At low densities these chains form an isotropic phase, whereas, at high densities, these particular DNA solutions are known to order into the nematic liquid crystal phases. Here, we put forward a theoretical approach, which suggests how to predict the average chain length and the stacking free energy, based on the experimental scattering patterns. We show that the proposed method is rather general and might be used for any self-assembling anisotropic particles, as long as the chain-size distribution is exponential.

CPP 11.14 Mon 17:30 Poster C

Dissociation behavior of pyridine coordination compounds in aqueous solutions — ●MANUEL GENSLER¹, CHRISTIAN EIDAMSHAUS², ARTUR GALSTYAN², ERNST-WALTER KNAPP², HANS-ULRICH REISSIG², and JÜRGEN P. RABE¹ — ¹Institut für Physik, Humboldt-Universität zu Berlin — ²Institut für Chemie und Biochemie, Freie Universität Berlin

The pyridine core is ubiquitous in natural products and widely used for the construction of supramolecular structures [1]. We analyzed coordination compounds of mono- and bivalent pyridines with Cu(II) and Zn(II) by SFM based single molecule force spectroscopy (SMFS) in aqueous solutions. Using the Bell-Evans-Kramers model we determined surprisingly long rupture lengths from 0.25 nm for the monovalent pyridin with Cu(II) up to 0.52 nm for the bivalent pyridine with Cu(II). DFT calculations suggest a stepwise dissociation through an intermediate product in which a water ligand inserts in between the pyridine and metal ion. Such process is different to the known solvent-ligand-exchange mechanism of a pyridine-palladium complex in DMSO with a rupture length of only 0.17 - 0.19 nm [2]. Therefore additional water ligands may attribute to the mechanical properties of metallosupramolecular compounds and their corresponding natural systems.

[1] L.E. Kapinos and H. Sigel *Inorg. Chim. Acta* **2002**, *337*, 131-142. [2] F.R. Kersey et al. *J. Am. Chem. Soc.* **2006**, *128*, 3886-3887.

CPP 11.15 Mon 17:30 Poster C

Probing the electronic structure of gas phase methanol by soft RIXS — ●ANDREAS BENKERT^{1,2,3}, FRANK MEYER¹, MONIKA BLUM⁴, REGAN G. WILKS⁵, MARCUS BÄR^{4,5}, WANLI YANG⁶, FRIEDRICH REINERT^{2,3}, CLEMENS HESKE^{1,4,7}, and LOTHAR WEINHARDT^{1,4,7} — ¹Inst. for Photon Science and Synchrotron Radiation, Karlsruhe Institute of Technology (KIT) — ²Exp. Physik VII, Universität Würzburg — ³Gemeinschaftslabor für Nanoanalytik, KIT — ⁴Dept. of Chemistry, University of Nevada, Las Vegas — ⁵Solar Energy Research, Helmholtz-Zentrum Berlin f. Mat. u. Energie — ⁶Advanced Light Source, Lawrence Berkeley National Laboratory — ⁷ANKA Synchrotron Radiation Facility Karlsruhe, KIT

We have investigated methanol in gas phase at atmospheric pressure using resonant inelastic soft x-ray scattering (RIXS). RIXS maps of both, the O K and C K edge, will be presented, and it will be shown that the observed emission lines can be attributed to different molecular orbitals in accordance to DFT-based calculations of isolated methanol molecules. This demonstrates the local character of the RIXS process.

In detail, we observe strong spectator shifts of up to 0.9 eV upon excitation into different absorption resonances at the O K edge. Furthermore, we find evidence for nuclear dynamics on the time scale of the x-ray emission process, leading to a dissociation of the hydrogen atom from the hydroxyl group. In addition, measurements of deuterated methanol allow us to separate the contributions of intact and dissociated methanol molecules in the emission spectra.

CPP 12: Poster: Nanoparticles and Composite Materials

Time: Monday 17:30–19:30

Location: Poster C

CPP 12.1 Mon 17:30 Poster C

Experimental Observation of the wetting property of homopolymer on a grafted polymer on a curved substrate — ●CHANG JONG KIM¹, MARKUS MAZUROWSKI², JUN YU LI¹, MARKUS GALLEI², KATRIN SONDERGELD², HENNRICH FRIELINGHAUS³,

MATTHIAS REHAHN², and BERND STÜHN¹ — ¹Experimental Condensed Matter Physics, TU Darmstadt — ²Ernst-Berl-Institute for Technical and Macromolecular Chemistry, TU Darmstadt — ³Jülich Centre for Neutron Science, Forschungszentrum Jülich GmbH

The wetting property of homopolymer on a grafted polymer on a nanoparticle surface is greatly influenced by the ratio of the molar mass of the polymer on the surface (N) and the matrix polymer (P). Grafting density and the ratio of the length of grafted polymer (R_g) to the radius of a core (R_c) may play an important role in the wetting property as well. The change of the wetting property, the wetting-dewetting transition, is therefore expected to be induced by a combination of three parameters: P/N, R_g/R_c ratio and grafting density. In our experiment, Polystyrene (PS) was grafted from the surface of nanoparticles (silica and deuterated PS). These particles were then dispersed in deuterated PS matrices and measured by Small Angle X-ray Scattering (SAXS) and Small Angle Neutron Scattering (SANS). P/N ratio was varied from <1 to $\gg 1$ and R_g/R_c ratio was tuned by using two different molar masses of the grafted chain onto which the same core was used. In particular the analysis of the SANS results allows to determine thickness and conformation of the polymer brush on the curved substrate.

CPP 12.2 Mon 17:30 Poster C

Electrochemical Approach to Control CdSe/ZnS Quantum Dot Fluorescence — •DAVID PLOTZKI, NICOLE AMECKE, and FRANK CICHOS — Molecular Nanophotonics Group, University of Leipzig

The fluorescence behaviour of colloidal semiconductor nanocrystals can be tuned by adjusting the electric conditions of their close environment. We aim to electrochemically manipulate the charge concentration on the nanocrystal surfaces in order to alter the occupancy of trap states. Recent research indicates that such surface traps strongly influence nonradiative decay channels.

We investigate single colloidal CdSe/ZnS Quantum Dots on ZnO-coated ITO surfaces. Using a confocal microscope setup with the ability to study lifetimes and spectra, we explore the fluorescence behaviour under specific electrochemical potentials.

From ensemble as well as single QD measurements we find potential ranges where the nanocrystal fluorescence is either enhanced or suppressed, accompanied by a decrease or increase of the total non-radiative decay rate. Additionally, sudden potential changes cause a delayed fluorescence response. These results hint at a rearrangement of the occupancy of trap states.

CPP 12.3 Mon 17:30 Poster C

Influence of gold nanoparticle distributions on SERS enhancement factors — •THOMAS SANDER¹, HONGMEI LIU², XINPING ZHANG², and PETER J. KLAR¹ — ¹I. Physikalisches Institut, Justus-Liebig-Universität Giessen — ²College of Applied Sciences, Beijing University of Technology

Surface enhanced Raman spectroscopy (SERS) of metallic nanostructured substrates can provide Raman intensities increased by several orders of magnitude making even the detection of single molecules possible. Two different mechanisms contribute to the enhancement of the Raman signals: The electromagnetic enhancement is due to excited surface plasmons of the metal structure causing locally increased electromagnetic fields. The chemical enhancement is due to various effects, e.g. the chemical interaction between the molecules and the surface.

Here we present Raman spectra of rhodamine 6G on gold nanostructures fabricated by solution processible gold nanoparticles on Si substrates. The properties of the gold nanostructures can easily be varied by annealing at different temperatures as shown by AFM and SEM. A gold coordinate grid on the Si substrate allows one to correlate the recorded Raman spectra with the AFM and SEM measurements. Thus the influence of the gold nanoparticle distribution on the signal enhancement is accessible in detail. Raman spectra will be discussed with respect to different excitation lasers and polarizations as well as the achieved enhancements with respect to the local environment of the gold nanoparticles. COMSOL simulations of the enhancement factors will be compared with the experimental results.

CPP 12.4 Mon 17:30 Poster C

Optical switchable properties of polymer-carbon-nanotubes nanocomposites based on photochromic molecules — •VIKTOR SCHNEIDER¹, THOMAS STRUNSKUS¹, MADY ELBAHRI², and FRANZ FAUPEL¹ — ¹Technische Fakultät der Uni Kiel, Institut für Materialwissenschaft-Materialverbunde — ²Technische Fakultät der Uni Kiel, Institut für Materialwissenschaft-Nanochemistry and Nano-engineering

Photochromic molecular switches are a class of organic molecules that

allow a reversible control over the molecular structure or the molecular dipole moment with light. This attributes provide the possibility of photoswitching of bulk properties of composite materials like electrical conductance or dipole moment. In this work, azobenzene based chromophores were incorporated into polymer-carbon-nanotubes nanocomposites, and the photoswitching properties were investigated in a self made electro-optical measuring station. The changes in electrical resistance by illumination with ultraviolet (360 nm) and blue light (480 nm) were measured. For the multi wall carbon nanotubes, switching amplitudes of several percent were achieved, while single wall carbon nanotubes showed even changes up to 30 percent in resistance. The switching and conductance change mechanisms will be discussed.

CPP 12.5 Mon 17:30 Poster C

Synthesis and characterization of silica-encapsulated Ni nanorods — •FLORIAN KRÄMER, ANDREAS TSCHÖPE, and RAINER BIRINGER — Universität des Saarlandes, Saarbrücken

Ni nanorods are uniaxial ferromagnetic particles which can be used in nanorheology to probe local viscoelastic properties of soft matter. The present study is focused on the encapsulation of the nanorods by a silica layer which provides a well-defined interface for subsequent surface functionalization. Alumina templates with hexagonally arranged pores were synthesized by two step anodization of aluminum. The alumina-layer was separated by a voltage reversal technique. The barrier oxide at the pore-bottom was dissolved by chemical etching resulting in free-standing mesoporous membranes with completely open pore morphology. The whole surface of the membrane including the porewalls was coated with a thin silica layer by atomic layer deposition. Ni nanorods were synthesized by direct current electro-deposition of Ni into the pores. The filled templates were characterized by static magnetization measurements revealing a coercivity of $\mu_0 H_C = 56$ mT. Afterwards the rods were released from the template by dissolution of the alumina in NaOH. Transmission electron microscopy revealed a rod diameter of 60 nm and a thickness of the silica layer of 3 nm. The anisotropic optical properties of the rods which are the physical basis for magneto-optical rheometry, were investigated with regards to the influence of the silica layer and the size of the nanorods.

CPP 12.6 Mon 17:30 Poster C

Sol-Gel Templated Zinc Oxide Films for Applications in Hybrid Photovoltaics — •ERIK BRADEN, KUHU SAKAR, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany

In recent years a broad field of research concerning hybrid solar cells has been developed as they show a high potential to become an important source of green energy. Hybrid solar cells consist of an inorganic electron acceptor and an organic hole-conductor. In the present study, zinc oxide is utilized as the inorganic material in the form of nanostructures. Zinc oxide (ZnO) nanostructures are synthesized on silicon substrates forming grid-like morphology. The synthesis is done by using a sol-gel mechanism coupled with an amphiphilic diblock copolymer poly(styrene-block-4-vinyl pyridine) P(S-b-4VP), acting as a template. The morphology is synthesized by using zinc acetate dihydrate (ZAD) as a suitable commercial ZnO precursor on silicon (100) substrates using different deposition techniques. This involves spin-coating, spray-coating, dip-coating, blade-coating and solution casting. It is tried to produce a homogenous film with a certain thickness range between 300 nm and 500 nm which is expected to be most favorable for the solar cell performance. The influences of the different coating techniques on the morphology are investigated by optical microscopy, scanning electron microscopy (SEM) and atomic force microscopy (AFM). The thickness is measured with white light interferometry and height profilometry. An overview about the surface roughness of the films is obtained via atomic force microscopy (AFM).

CPP 12.7 Mon 17:30 Poster C

Thermal and mechanical properties of styrene butadiene rubber/alumina nanocomposites — •RYMMA SUSHKO, JÖRG BALLER, MARLENA FILIMON, and ROLAND SANCTUARY — Laboratory for the Physics of Advanced Materials, University of Luxembourg, 162a avenue de la Faucellerie, L-1511, Luxembourg

SBR is a rubber material with high technical relevance. In order to enhance the mechanical properties of the rubber we dispersed inorganic nanoparticles in the polymer matrix. By doing so, the properties of a given composite can be tuned either by changing the nanoparticle concentration or by modifying the surface properties of the fillers. Both interventions have indeed the potential to take influence on the struc-

ture and properties of the interphases emerging between the fillers and the polymer matrix. In this contribution we report on the glass transition behavior of SBR/alumina nanocomposites when the concentration and surface properties of the alumina nanoparticles are changed. We also discuss the influence of the fillers on the shear stiffness of the rubber material. The samples were investigated by TMDSC and DMA methods. TMDSC investigations shed light on a surprising behavior of the glass transition temperature when the nanoparticle concentration is changed: at low filler contents the glass transition temperature T_g passes through a minimum. While further increasing the nanoparticle content T_g increases to finally saturate at high concentrations. One of the main DMA results is that increasing of the alumina concentration induces a quasi-solid-like frequency-independent response of the nanocomposites in the low frequency regime.

CPP 12.8 Mon 17:30 Poster C

Novel approach for the rapid thermal processing of polymer-metal composites using 2.45 GHz microwave radiation — ●ANDREAS WURM¹, RADU NICULA², KOTARO ISHIZAKI², MANUELA STIR², SEBASTIEN VAUCHER², EVGENY ZHURAVLEV¹, and CHRISTOPH SCHICK¹ — ¹University of Rostock, Institute of Physics — ²Swiss Federal Laboratories for Materials Science and Technology - Empa, Advanced Materials Processing

In contrast with traditional polymer melt-processing methods, new opportunities for improved material properties are sought by various R&D and industrial groups through the use of powder processing technologies, in particular for polymer-matrix composites. For example, in the field of new biomaterials for acetabular cup prosthetics, UHMWPE composites comprising AlCuFe quasicrystalline (QC) particles were shown to exhibit significantly improved wear loss properties compared to pure UHMWPE or Al₂O₃/UHMWPE composites, without losing the excellent biocompatibility of the UHMWPE matrix. Further improvement of the wear resistance of such composite materials is nowadays sought in the better anchoring of the metal particles to the polymer matrix. Towards this objective, a novel rapid thermal processing approach is proposed that mainly exploits the selective absorption of microwave field energy by the metal particle constituent of the composite material.

CPP 12.9 Mon 17:30 Poster C

Fast Spectral Analysis of Quantum Dot Blinking — ●CLEMENS GÖHLER, CORNELIUS KRASSELLT, and CHRISTIAN VON BORCZYKOWSKI — Chemnitz University of Technology, Institute of Physics, Germany

While investigating individual semiconductor nanocrystals (quantum dots, QDs) using single molecule techniques, photoluminescence intermittency (blinking) can be observed. This means emission is temporarily suppressed under constant excitation. This behaviour can be explained by a trapping model, assuming electron and hole to be localised in trap-states in QD interfaces or the environment [1].

It has been shown that a two-level-system with on- and off-intensity does not exactly describe the blinking process since experiments imply the existence of intermediate intensities as well [2]. According to the trapping model, this may refer to a hole-trapping mechanism. Additionally, the localised charge will influence the recombination process due to the quantum-confined Stark effect, resulting in spectral shifts within the photoluminescence.

In our experiments we investigate this spectral diffusion in relation to the intermediate intensities. Confocal microscopy is used to detect photoluminescence light from single ZnS/CdSe QDs. Moreover, emission light is separated onto two individual photodiodes by passing a dichroic beam splitter and the intensity levels are determined from recorded photon arrival times using a Change-Point-Algorithm.

[1] F. Cichos, C. von Borczykowski, M. Orrit: COCIS 12(2007), 272.

[2] R. Schmidt, C. Krasselt, C. von Borczykowski: Chem. Phys. 406(2012), 9.

CPP 12.10 Mon 17:30 Poster C

Morphology studies for titania nanoparticle based hybrid solar cells — ●STEPHAN PRÖLLER, VOLKER KÖRSTGENS, and PETER MÜLLER-BUSCHBAUM — TU München, Physik Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany

Thin films containing titania nanoparticles have a variety of applications. For applications in photovoltaics a high absorption coefficient and a large surface area are desirable. Blends of organic and inorganic semiconductors are denoted as hybrid solar cells. Those hybrid solar cells combine the advantages of inorganic semiconductors with the

film-forming polymer. Properties of inorganic nanoparticles are size tunability, high absorption coefficients and high mobilities. We use nanoparticles as acceptors in polymer-titania hybrid solar cells. Furthermore, we investigate the influence on the performance of solid-state dye sensitized solar cells based on ruthenium dye and spiro-OMeTAD as hole transport material. The thin films are prepared via spin-coating and solution casting, respectively. The surface structure is investigated with SEM. Thickness and structure of the layer are studied with XRR, the optical properties with UV/Vis spectroscopy and the efficiency of the different solar cells is measured under AM 1.5 conditions.

CPP 12.11 Mon 17:30 Poster C

Thin films of sponge-like titania nanostructures with controllable thickness — ●LIN SONG, MARTIN A. NIEDERMEIER, and PETER MÜLLER-BUSCHBAUM — TU München, Physik Department, LS Funkt. Mat., James-Frank-Str. 1, 85748 Garching, Germany

Titania nanostructures have a huge application potential, e.g. in photovoltaics, photocatalysis and gas sensing. For all these applications, a high surface area is important. Sponge-like titania nanostructures are especially promising due to their morphology with a high surface area and an interconnected network. The titania nanostructures are prepared from block copolymer templating in combination with sol-gel chemistry. The templated titania sol-gel is deposited on a substrate by spin-coating, via calcination the polymer template is combusted and nanostructured crystalline titania thin films are obtained. Additionally, the sol-gel approach allows for a control of the film thickness. The surface morphology is investigated with scanning electron microscopy (SEM) and optical microscopy (OM), the optical properties and the film thickness are probed with UV/Vis spectroscopy and ellipsometry.

CPP 12.12 Mon 17:30 Poster C

Ultrafast Spectroscopy of excitonic states in an individual CdSe nanowire — ●THORSTEN SCHUMACHER^{1,2}, HARALD GIESSEN², and MARKUS LIPPITZ^{1,2} — ¹Max Planck Institute for Solid State Research, Stuttgart — ²4th Physics Institute, University of Stuttgart

We investigate the spectrally resolved ultrafast carrier dynamics of excitonic states of a single CdSe nanowire at room temperature. The transient absorption spectra show characteristic short and long living effects that we attribute to a highly excited electron-hole plasma and excitonic state bleaching. We discuss both phenomena and show a very good agreement between the detected bleaching signal and the dipole allowed excitonic transition energies, calculated by a six band-effective mass model. Furthermore we extract the lifetime of various transitions and set them in comparison to the corresponding photoluminescence response. Here we obtain hints on radius fluctuations within a single wire leading to an enhanced probability of spontaneous emission at these large radius defects.

CPP 12.13 Mon 17:30 Poster C

Analyzing the electrical properties of percolating carbon nano-tubes or nano-fibers in composite-materials — ●MICHAEL KONTER¹, PABLO CARBALLEIRA², BERND WETZEL², and ROLF PELSTER¹ — ¹Fachrichtung 7.2 Experimentalphysik, Universität des Saarlandes, Saarbrücken, Germany — ²Institut für Verbundwerkstoffe GmbH, Kaiserslautern, Germany

We compare different types of composite materials containing carbon nano-fibers (CNF) or carbon nano-tubes (CNT) with fillings ranging from 0-2%. These were dispersed in an epoxy resin either with a three roll calendar device or with a torus mill laboratory mixing device. After polymerization solid samples are obtained that were characterized via temperature dependent dielectric spectroscopy (10 Hz - 2 GHz, 40 K - 290 K). For samples above the percolation threshold ($f_c = 0,08\text{vol.}\%$) we observe a broad polarization process, that is correlated with the dc-conductivity. An effective medium analysis reveals several intrinsic parameters. Here we discuss (i) the ratio of the inter-fiber or inter-tube contact resistance to the intrinsic resistance, $R_{\text{contact}}/R_{\text{carbon}}$ and (ii) the product of percolation strength and intrinsic CNT or CNF conductivity, $C \cdot \sigma_{\text{carbon}}$, as well as its activation energy. The data reveals the quality of the inter-fiber contacts and thus reflects differences in the sample preparation.

CPP 12.14 Mon 17:30 Poster C

Structure-Property relationships of Nanocomposites Based on Polylactide and Layered Double Hydroxides — ●JING LENG¹, PURV PUROHIT¹, DE-YI WANG^{2,3}, and ANDREAS SCHOENHALS¹ — ¹BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany — ²Madrid Insti-

tute for Advanced Studies of Materials, C/Eric Kandel 2, 28906 Getafe, Madrid, Spain — ³Center for Degradable and Flame-Retardant Polymeric Materials (ERCEPM-MoE), College of Chemistry, Sichuan University, Chengdu 610064, China

Abstract: Polymer based nanocomposites prepared by melt blending of synthesized NiAl layered double hydroxides (NiAl-LDH) and polylactide (PLA) were investigated by combination of differential scanning calorimetry (DSC), small- and wide-angle X-ray scattering (SAXS and WAXS) and broadband dielectric spectroscopy (BDS). In the case of NiAl-LDH based nanocomposites the degree of crystallinity at first increases and then decreases as a function of LDH concentration. By extrapolation a limiting concentration of NiAl-LDH ca.15% where the crystallization of PLA is completely suppressed by the nanofiller. The dielectric spectra of the nanocomposites show several relaxation processes related to dynamic glass transition and localized fluctuations were identified and analyzed in detail to understand the morphology. The results of the PLA based nanocomposites with NiAl-LDH as nanofillers were further compared with PLA based nanocomposites with MgAl-LDH as nanofillers.

CPP 12.15 Mon 17:30 Poster C

Ultrafast strain-mediated response of functionalized polyelectrolyte nanolayers — ●STEFFEN MITZSCHERLING — Universität Potsdam

We prepared layered functional nanostructure samples by spin-assisted layer-by-layer deposition of polyelectrolytes. In analogy to our previous study on spherical gold nanoparticles we show that gold nanorods exhibit even larger spectral shifts and amplitude variations when their dielectric environment is modified.[1,2]

We use the plasmon resonance of the metallic particles to detect ultrashort strain pulses travelling through polymeric layer structures. These hypersound waves are generated by excitation of azobenzene-containing layers. We characterize the strain pulse by ultrafast broadband Brillouin-scattering [3] in order to derive conclusions on the actuation and nonlinear propagation in such complex polymeric nanolayer systems.

[1]Kiel et al., Langmuir, 28, 4800 (2010).

[2]Kiel et al., Langmuir, 26, 18499 (2012).

[3]Bojahr et al., Physical Review B, 86, 144306 (2012).

CPP 12.16 Mon 17:30 Poster C

Analysis of Particle-Particle Interaction Potentials in Aqueous Nanoscale Systems — ●JULIAN SCHULZE¹, MICHAEL PAULUS¹, JOHANNES MÖLLER¹, METIN TOLAN¹, and ROLAND WINTER² — ¹Fakultät Physik / DELTA, Technische Universität Dortmund, 44221Dortmund, Germany — ²Fakultät Chemie, Technische Universität Dortmund, 44221 Dortmund, Germany

In previous studies small angle X-ray scattering (SAXS) was used to study the interaction potential of proteins in aqueous solution under the influence of varying conditions such as pressure, temperature or further cosolvents. A non-linear correlation between the strength of the protein-protein interaction and hydrostatic pressure was found with a minimum at 2 kbar. Adding salts led to a linear increase of the attractive part of the interaction potential, while adding Trimethylaminoxid (TMAO) causes a shift of the minimum to higher pressures. In the presented work the pressure dependent behavior of the interaction potential of nano particles is determined by SAXS. Furthermore, the pressure dependent structure of the solvent is explored by wide angle X-ray scattering (WAXS). Spherical nanoparticles are used because their structure factor is easy to model. Besides the WAXS data is not influenced by the scattering signal from the complex inner structure of proteins, so that changes of the water structure factor can be determined.

CPP 12.17 Mon 17:30 Poster C

Spectroscopic Ellipsometry of Anisotropic Nanocomposites — ●JOHANNES F. H. RISCH¹, BASTIAN BESNER², MARYAM HASHEMI², MATTHIAS SCHWARTZKOPF¹, ADELIN BUFFET¹, BERIT HEIDMANN¹, GERD HERZOG¹, VOLKER KÖRSTGENS³, EZZELDIN METWALLI³, JAN PERLICH¹, ANDRE ROTHKIRCH¹, MONIKA RAWOLLE³, KAI SCHLAGE¹, PETER MÜLLER-BUSCHBAUM³, RALF RÖHLSBERGER¹, RAINER GEHRKE¹, MICHAEL A. RÜBHAUSEN², and STEPHAN V. ROTH¹ — ¹DESY, Hamburg, Germany — ²Uni. Hamburg, Institut für Angewandte Physik, Hamburg, Germany — ³TU München, Physik Department E13, Garching, Germany

Optical anisotropic thin films have a wide field of application like an-

tenna, sensors or LEDs. Vacuum sputter deposition, which is commonly used in industry has been proven a reliable method for preparing thin films. Glancing angle deposition (GLAD) [1] of gold on top of a colloidal array of polystyrene nanospheres was used to create anisotropic optical properties in nanocomposite thin films. Using spectroscopic ellipsometry, we investigated the change of optical properties caused by asymmetric deposition of gold clusters. Since commercial standard software does not enclose applicable fitting models, a new analyzing software is developed fulfilling the complex demands to model anisotropic media. In order to extract the optical response of each active layer, a systematic sample analysis comprising the measurements of single components of GLAD samples was performed. As a result, an energy depending change of azimuthal symmetry is observed. [1] Gonzalez-Garcia et al., ChemPhysChem 11, 2005 (2010)

CPP 12.18 Mon 17:30 Poster C

Spectroscopic Ellipsometry of Anisotropic Nanocomposites — ●JOHANNES F. H. RISCH¹, BASTIAN BESNER², MARYAM HASHEMI², MATTHIAS SCHWARTZKOPF¹, ADELIN BUFFET¹, BERIT HEIDMANN¹, GERD HERZOG¹, VOLKER KÖRSTGENS³, EZZELDIN METWALLI³, JAN PERLICH¹, ANDRE ROTHKIRCH¹, MONIKA RAWOLLE³, KAI SCHLAGE¹, PETER MÜLLER-BUSCHBAUM³, RALF RÖHLSBERGER¹, RAINER GEHRKE¹, MICHAEL A. RÜBHAUSEN², and STEPHAN V. ROTH¹ — ¹DESY, Hamburg, Germany — ²Uni. Hamburg, Institut für Angewandte Physik, Hamburg, Germany — ³TU München, Physik Department E13, Garching, Germany

Optical anisotropic thin films have a wide field of application like antenna, sensors or LEDs. Vacuum sputter deposition, which is commonly used in industry has to be proven a reliable method for preparing thin films. Glancing angle deposition (GLAD) [1] of gold on top of a colloidal array of polystyrene nanospheres was used to create anisotropic optical properties in nanocomposite thin films. Using spectroscopic ellipsometry, we investigated the change of optical properties caused by asymmetric deposition of gold clusters. Since commercial standard software does not enclose applicable fitting models, a new analyzing software is developed fulfilling the complex demands to model anisotropic media. In order to extract the optical response of each active layer, a systematic sample analysis comprising the measurements of single components of challenging GLAD samples was performed. As a result, an energy depending change of azimuthal symmetry is observed. [1] Gonzalez-Garcia et al., ChemPhysChem 11, 2005 (2010)

CPP 12.19 Mon 17:30 Poster C

OLED structures utilizing silicon nanoparticles — HANS VOLKER STEGEMANN¹, ●JENS THEIS¹, AXEL LORKE¹, and HARTMUT WIGGERS² — ¹Fakultät für Physik and CENIDE, Universität Duisburg-Essen — ²Institut für Verbrennung und Gasdynamik and CENIDE, Universität Duisburg-Essen

We have fabricated electroluminescence devices based on silicon nanoparticles (Si-NP) and conducting polymers. The Si-NPs have been synthesized from the gas phase in a low-pressure microwave plasma using SiH₄ as a precursor.

Two different sample designs were developed and characterized. For the first kind of samples, the NPs were embedded in a layer structure consisting of hole-conducting and electron-conducting polymers. For electrical contact an evaporated silver film was used as cathode and a transparent indium tin oxide (ITO) coated glass slide as anode. For the second sample structure, the NPs were embedded between two electrodes in a conducting polymer matrix. Here ITO/glass was used as anode. For the cathode different metals have been employed to investigate their influence on the luminescence.

Carrying out electroluminescence measurements, we obtain visible light emission for both sample structures. The spectra showed two broad bands which could be identified by additionally performed PL-measurements as the emission from the Si-NPs and the polymers, respectively.

CPP 12.20 Mon 17:30 Poster C

Photoluminescence of CdSe, Au and Hybrid Nanoparticle Systems — ●DANIEL BRAAM¹, ZHENG MA¹, PIN-WEN WANG^{1,2}, JENS THEIS¹, GÜNTHER M. PRINZ¹, PHILIPP WAGENER³, STEPHAN BARCIKOWSKI³, and AXEL LORKE¹ — ¹Fakultät für Physik and CENIDE, University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany — ²Harvard School of Engineering and Applied Sciences Pierce Hall 29 Oxford Street Cambridge, MA 02138, USA — ³Fakultät für Chemie and CENIDE, University of Duisburg-Essen,

Universitätsstraße 7, 47057 Duisburg, Germany

Gold and Gold/Silver nanoparticles were fabricated with laser ablation and characterized with SEM, TEM, UV/VIS and photoluminescence measurements. They show a large size distribution and agglomeration, as well as a broad PL signal, which results from the decay of a particle plasmon within the model of Dulkeith et al [1]. Continuous excitation with a 405nm diode laser steadily shifts the peak wavelength to lower energies and reduces the intensity, which regenerates to some extent after exposure. In a second step we examine the interaction between metal and semiconductor nanoparticles by adding CdSe/ZnS quantum dots to the Au and Au/Ag NP solutions. First spectrum and peak analysis show mixed emission, which can be explained by a simple superposition of the Au and the CdSe NP PL. No indication of interaction between metallic and semiconductor nanoparticles is observed in the emission energies, presumably due to insufficient mixing, leading to a large distance between both components.

[1] E. Dulkeith et al., PRB **70**, 205424 (2004)

CPP 12.21 Mon 17:30 Poster C

AFM and physicochemical characterization of Upconversion Nanoparticles — ●HEBA S. MOHAMAD¹, PETER NESTLER¹, HARM WULFF¹, STEFANIE PERFAHL², PATRICK BEDNARSKI², and CHRISTIANE A. HELM¹ — ¹Inst. für Physik, Uni Greifswald, D-17487 Greifswald — ²Inst. für Pharmazie, Uni Greifswald, D-17487 Greifswald

Recently, the development of upconversion nanoparticles (UCNPs) for fluorescence imaging and drug delivery monitoring attracted attention. For biological labeling, cancers diagnosis and detection, NaYF₄O:Yb,Er is a promising candidate. The sequential absorption of two or more photons in the near infrared (NIR) leads to an emission in the visible range. The NaYF₄O:Yb,Er nanoparticles aggregate in water. Therefore their surface is modified using different approaches. Since the upconversion depends strongly on the crystallographic structure of the UCNPs (either cubic or hexagonal), the ratio of both species within an adsorbed layer needs to be optimized to improve the upconversion property. Main goals of this investigation are formation of homogeneous and well distributed UCNPs layers, to examine the upconversion properties.

To determine the size of UCNPs, Atomic Force Microscopy (AFM) is used. The crystalline structure is characterized by the X-ray diffraction (XRD) pattern, to correlate optical with crystallographic properties. The absorption properties are determined with UV-Vis absorption spectroscopy. With a 980 nm laser excitation source the upconversion properties are investigated.

CPP 12.22 Mon 17:30 Poster C

Correlation of optical characteristics of gold nanoparticle-DNA networks with size and internal structure — ●MALTE LINN¹, ANNE BUCHKREMER², JAN TIMPER³, THOMAS ECKERT⁴, WALTER RICHTER⁴, JOACHIM MAYER³, GERO VON PLESSEN¹, and ULRICH SIMON² — ¹Inst. of Physics (IA), RWTH Aachen University — ²Inst. of Inorganic Chemistry, RWTH Aachen University — ³Central Facility for Electron Microscopy, RWTH Aachen University — ⁴Inst. of Physical Chemistry, RWTH Aachen University

The application of nanoplasmonic materials relies on the fabrication of metallic nanostructures with well defined sizes and geometries. By mixing different ratios of DNA-functionalized gold nanoparticles (AuNPs), various kinds of DNA-AuNP networks can be tailored. The size and internal structure of these networks determines their optical properties, due to interparticle coupling. The networks are thermally and photothermally addressable and therefore interesting for possible applications in the fields of drug release or gene regulation. In this work, we analyze the size and internal structure of DNA-AuNP networks by combining optical extinction spectroscopy, dynamic light scattering, small angle X-ray scattering, in situ-TEM measurements and generalized Mie calculations. Using these techniques, we determine the different interparticle distances in the networks. For small networks, they are consistent with a center-shell geometry.

CPP 12.23 Mon 17:30 Poster C

Broadband Dielectric Spectroscopy and Rheology on Polyisoprene Silica Nanocomposites — ●ADRIAN HAMM¹, GERALD J. SCHNEIDER², LUTZ WILLNER¹, WIM PYCKHOUT-HINTZEN¹, REINER ZORN¹, and DIETER RICHTER¹ — ¹Jülich Centre for Neutron Science JCNS-1, Jülich, Deutschland — ²Jülich Centre for Neutron Science JCNS-FRM-II, Garching, Deutschland

Even though polymer nanocomposites have been playing a crucial role

in our daily life for many years, the microscopic origin of the material properties is not fully understood. Therefore, we performed dielectric spectroscopy and rheology experiments on simple model-like polyisoprene silica nanocomposites.

In general, the response of polymer melts to an external perturbation, such as an electric field or a mechanical stress, causes a signal that depends on the sample and on the method. Even in case of identical samples, the measured relaxation function can be different and thereby reveal different details on the molecular origin of the measured values. In our contribution, we demonstrate how to ascribe the different relaxation functions measured by rheology and by broadband dielectric spectroscopy in nanocomposites to the different origins inherent with the different methods.

CPP 12.24 Mon 17:30 Poster C

Computational Simulation of Molecular Motors — ●ABBAS ALI DEHGHAN BAGHI — Ruhr-University Bochum, Bochum, Germany

We have used molecular mechanics simulations based on Force Field methods to study the molecular systems which would be able to perform a rotation motion. The research intends to understand the fundamental principles of these molecular motions. We used classical simulations methods by using TINKER package to optimize such molecular systems and do the basic analysis of these systems. But, we have checked our results with quantum chemistry calculations methods. The *ab initio* electronic structure calculations were performed using the TURBOMOLE package where DFT calculations have been done on the B97-D (GGA) level with Triple-Zeta Valence Plus Polarization (TZVPP) basis sets and the dispersion correction in the package is based on the atom-pair wise DFT+D2 level. We have focused on the binding energy of the molecular structures as a key factor to our analysis on both classical and quantum chemistry methods. We are interested in supramolecular motors whose stator and rotor are not covalently attached to each other, but are held mechanically and act like a "Ball and Bowl" which rotate without axle to each other. The fullerene C₆₀ corresponds to the ball and is referred as a guest and Tribenzotriquinacen molecule corresponds to the Bowl and is referred as a host. We have investigated that the interaction between the host and the guest is solely due to dispersive interactions which has been certified by a negligible charge transfer from the host to the guest C₆₀ upon binding and such systems are among physisorption systems.

CPP 12.25 Mon 17:30 Poster C

Surfactant modified silica particles at the air/water interface — ●ADRIAN CARL, ANNE BANNUSCHER, and REGINE VON KLITZING — TU Berlin, Straße des 17. Juni 124, Institut für Physikalische Chemie, Stranski Laboratorium

The combination of nanoparticles and suitable surfactants has been shown to increase aqueous foam stability compared to the same system without nanoparticles. The origin of the increased stability is not fully resolved, yet. Unmodified, hydrophilic nanoparticles show no attachment to the water/air interface. On addition of surfactant, the particles are rendered hydrophobic and adsorb to the interface. In equilibrium, a specific surface coverage is obtained. At the interface, a comparatively rigid particle layer, withstanding compression, is formed. The location within the interface is governed by the particle's wetting properties which are expressed by the contact angle.

We conduct x-ray reflectivity (XRR) measurements to characterize the equilibrium state of the adsorbed particle layer. The results are related to surfactant adsorption isotherms and the adsorption kinetics are obtained from dynamic surface tension measurements.

CPP 12.26 Mon 17:30 Poster C

Erbssenzählerei ? Wieso Nanopartikel gezählt werden müssen, und wie das gehen kann. — ●WENDEL WOHLLEBEN, JULES MIKHAEEL und VOLODYMYR BOYKO — BASF SE, Material Physics

Aufgrund der EU regulatorischen Definition von *Nanomaterial* müssen zehntausende von partikulären Produkten auf ihre Anzahlverteilung der enthaltenen Nanopartikel untersucht werden. Das trifft die Physik und Messtechnik unvorbereitet. Mit Ringversuchen und gezielten Validierungen wurden die Grenzen der Anwendbarkeit von etablierten und neuen Methoden ausgelotet.[1] Einzelpartikel- und Fraktionierungs-Methoden wie NTA, EZS, FFF, AUC haben Vorteile bei den inhomogenen, polymorphen, durch Wechselwirkung mit ihrer Umgebung veränderten Materialien[2,3], können aber oft Partikel unter 20nm oder über 1µm nicht erfassen. Streu-Methoden wie DLS oder SLS scheitern an der Polydispersität, andere wie AFM und TEM-Tomographie sind statistisch nur marginal belastbar. Eine regelrechte

Messstrategie muss mit 1D, 2D und 3D Nanomaterialien validiert werden, bevor unbekannte Proben als regulatorisches Nanomaterial identifiziert werden können.

- [1] J. Nanopart. Res. (2012) DOI 10.1007/s11051-012-1300-z
- [2] Nanoscale (2012) DOI: 10.1039/c2nr32711b
- [3] ACS Nano 6 (2012) 4603

CPP 12.27 Mon 17:30 Poster C

Microscopic Investigation of Polymer Chain Dynamics in Nanocomposites with Strong Attractive Interaction — •THOMAS GLOMANN¹, GERALD J. SCHNEIDER², JÜRGEN ALLGAIER², and DIETER RICHTER² — ¹Jülich Centre for Neutron Science & Institute for Complex Systems, Forschungszentrum Jülich, 52425 Jülich, Germany — ²Jülich Centre for Neutron Science, Forschungszentrum Jülich, Outstation at FRM 2, Lichtenbergstraße 1, 85747 Garching, Germany

The mechanical properties of polymer based nanocomposites are essentially determined by surface interactions between the chains and filler particles. In particular the strong hydrogen bonding interaction energy causes dynamic adsorption of chain segments on hydrophilic surfaces which is often reported to yield an immobilized layer of mostly suppressed or “glassy” dynamics.

Using high-resolution quasi-elastic neutron scattering techniques we found experimental evidence for highly flexible chain dynamics within the adsorbed layers on both the large and local length scale. We present results of neutron spin-echo and time-of-flight measurements on PEO-Silica model systems where the interaction energy was tuned using differently terminated polymers.

CPP 12.28 Mon 17:30 Poster C

In-situ Synthesis of Semiconductor Nanoparticles Decorating Tubular J-aggregates — •YAN QIAO, FRANK POLZER, HOLM KIRMSE, EGON STEEG, STEFAN KIRSTEIN, and JÜRGEN P. RABE — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

Organic/inorganic hybrid nanomaterials, that combine the strengths of the individual organic and inorganic materials while compensating for their deficits, have recently attracted more and more attention. Quasi one-dimensional (1-D) nanomaterials, such as wires and tubes, have been intensively investigated owing to the benefit of dimensionality on electronic and optical properties [1]. Based on our previous results on silver [2], this work focuses on the fabrication of quasi 1-D organic/inorganic hybrid nanostructures consisting of nanotubular J-aggregates self-assembled from amphiphilic cyanine dyes, and semiconductor nanoparticles such as CdS decorating the surface of the nanotubes. Electrostatic interaction between the negative surface potential of the aggregates and the Cd²⁺ leads to the enrichment of Cd²⁺ within the ionic double layer close to the aggregate surface. Addition of thioacetamide leads to the formation of CdS nanocrystals with diameters less than 6 nm. With investigation of cryo-TEM and UV-Vis spectroscopy, it is found that CdS nanoparticles are exclusively formed at the surface of the aggregates. This opens a route to the formation of efficiently electronically coupled organic/inorganic systems.

- [1] Y. N. Xia et al., Adv. Mater. 2003, 15, 353.
- [2] D. M. Eisele et al., J. Am. Chem. Soc. 2010, 132, 2104.

CPP 12.29 Mon 17:30 Poster C

Tuning the electronic properties of the CuInS₂ nanoparticles for application in hybrid solar cells — •RANY MIRANTI¹, CHRISTOPHER KRAUSE¹, DOROTHEA SCHEUNEMANN¹, JOHANNES NEUMANN², DANIELA FENSKE², JOANNA KOLNY-OLESIAK¹, HOLGER BORCHERT¹, and JÜRGEN PARISI¹ — ¹Univ. of Oldenburg, Dept. of Physics, Energy and Semiconductor Research Laboratory, 26111 Oldenburg, Germany — ²Fraunhofer IFAM, Marie-Curie-Str.1-3 26129 Oldenburg, Germany

CuInS₂ (CIS) is one interesting material in solar cell applications because of the wide absorption range extending into the NIR and a lower toxicity. Despite much research in the CIS-based solar cells, the performance of CIS nanocrystal (NC) solar cells remains low so far. In case

of CIS/polymer bulk heterojunction solar cells the surface properties of the NCs are one important issue in this field. Modifying these surface properties is a promising method to influence the performance of the solar cells. Varying Cu to In precursor ratio in the synthesis leads to differences in the Cu and In concentrations in the CIS NCs' surfaces. CIS NCs prepared with Cu excess seem to accept more electrons than those with In excess. In the present work, CIS NCs were synthesized and characterized by XRD and TEM. Furthermore, we studied the composition of the NCs and the ligand shells by EDX and TGA, as well as the I-V characteristics in the hole and electron only devices. The influence of the Cu to In precursor ratio during the synthesis of CIS NCs on the performance of solar cells will also be discussed.

CPP 12.30 Mon 17:30 Poster C

Gold nanoparticles decorated with oligo(ethylene glycol) thiols: surface charges, and interactions with proteins in solution — •FAJUN ZHANG¹, MORITZ SCHOLLBACH¹, FELIX ROOSERUNGE¹, MAXIMILIAN W. A. SKODA², ROBERT M. J. JACOBS³, and FRANK SCHREIBER¹ — ¹IAP, Universität Tübingen — ²STFC, ISIS, Rutherford Appleton Laboratory, UK — ³University of Oxford, UK

We have studied the stability of OEG SAM decorated gold nanoparticles (AuOEG) and their interactions with proteins in solutions using DLS and zeta-potential measurements. We show that AuOEG particles carry a low net negative charge and are stable under a wide range of experimental conditions [1]. When mixed with proteins, negatively charged proteins do not adsorb to the colloid surface. However, with positively charged protein (lysozyme), zeta-potential values increase with protein concentrations and lead to a charge inversion, indicating adsorption of lysozyme to the colloid surface. The colloidal solutions become unstable near zero charge. Washing protein-bound colloids by centrifugation can remove only part of the adsorbed lysozyme. The effective charge inversion and rather strongly bound lysozyme on the colloid surface suggest that in addition to the charges formed at the SAM-water interface, there are defects on the surface of the colloid, which are accessible to the proteins [2]. The results of this study of surface charge, and stability shed light on the interaction with proteins of SAM coated AuNPs and their applications. [1] F. Zhang, et al. J. Phys. Chem. A 2007, 111, 12229. J. Phys. Chem. C 2009, 113, 4839. [2] M. Schollbach, et al. 2012, Submitted

CPP 12.31 Mon 17:30 Poster C

Optical and electrical properties of novel C₆₀/C₁₋₃ carbon cluster material. — •DMITRY STRELNIKOV and MANFRED M. KAPPES — KIT, Institute of Physical Chemistry II, Fritz-Haber-Weg 2, 76131 Karlsruhe

C₆₀ and C₁, C₂, C₃ clusters were co-deposited on SiO₂ substrate under high-vacuum conditions. Produced films were annealed to various temperatures up to 1200 K. Raman, UV-Vis spectra were measured ex-situ to characterize electronic and structural properties of the obtained carbon material. 4-point resistivity measurements were also performed. The obtained material may be interesting for carbon-based electronics.

CPP 12.32 Mon 17:30 Poster C

Fluorine patterning in C₂F_x determined by solid-state NMR and DFT — •ANASTASIA VYALIKH and ULRICH SCHELER — IPF Dresden

A combination of solid-state NMR and DFT has been used to elucidate the structure of room-temperature synthesized graphite fluorides C₂F_x intercalated with acetonitrile. 13C MAS NMR spectra confirm that all carbon sheets have been subjected to fluorination irrespective of the fluorination degree. However, the presence of graphite-like domains has been evidenced in the material with a low fluorination degree. By combining the 19F MAS NMR with DFT calculations, we demonstrate that all kinds of fluorine decoration patterns (isolated, end chain, mid-chain, cyclic and branched CF groups as well as infinite CF arrays and peripheral CF₂ defects) may exist in the low-temperature produced graphite fluorides. Analysing the data with different degree of fluorination, an evolution of fluorine patterns was proposed, involving CF chain formation and propagation towards the increasing chain length.

CPP 13: Biomaterials and Biopolymers I (joint session CPP/BP)

Time: Tuesday 9:30–13:00

Location: H34

Invited Talk

CPP 13.1 Tue 9:30 H34

Hierarchical Multi-Step Folding of Polymer Bilayers — GEORGI STOYCHEV^{1,2}, SEBASTIEN TURCAUD³, JOHN DUNLOP³, and ●LEONID IONOV¹ — ¹Leibniz Institute of Polymer Research Dresden, Hohestr. 6, 01069, Dresden, Germany — ²Technische Universität Dresden, Physical Chemistry of Polymer Materials, 01062, Dresden, Germany — ³Department of Biomaterials, Max Planck Institute of Colloids and Interfaces, Am Mühlenberg 1, 14424, Potsdam, Germany

We investigated the actuation of patterned bilayers placed on a substrate. We found that films display several kinds of actuation behavior such as wrinkling, bending and folding that result in a variety of shapes. Based on experiments and modeling, we argued that rectangular bilayers start to roll from the corners due to quicker diffusion of water. Rolling from long-side starts later and dominates at high aspect ratio[1].

It was also demonstrated that one can introduce hinges into the folded structure by proper design of the bilayers external shape without having to use site selective deposition of active polymers. Experimental observations lead us to derive four empirical rules backed up by theoretical understanding as well as simulations. We then demonstrated how those rules can be used to direct the folding of edge-activated polymer bilayers through a concrete example - the design of a 3D pyramid[2].

[1] Stoychev et al, "Hierarchical Multi-Step Folding of Polymer Bilayers", *Adv.Func.Mat.*, published online Nov 26, 2012

[2] Stoychev et al, "Shape-Programmed Folding of Stimuli-Responsive Polymer Bilayers", *ACS Nano*, 2012, 6(5), 3925-3934

CPP 13.2 Tue 10:00 H34

Mechanical properties of poly-L-lysine (PLL) / hyaluronic acid (HA) multilayer films measured by AFM — ●JOHANNES HELLWIG, CAGRI ÜZÜM, and REGINE VON KLITZING — Stranski-Laboratorium, Institut für Chemie, TU Berlin, Strasse des 17. Juni 124, 10623 Berlin, Germany

In recent years smart biomaterials have become a highly developing field of interest for biomedical applications, e.g. drug delivery. The layer-by-layer (LbL) technique gives the opportunity to build up self assembled polyelectrolyte multilayer films (PEM) with defined architecture, physical and chemical properties. PEM made of poly-L-lysine (PLL) and hyaluronic acid (HA) were produced by using the LbL technique. Potential applications of these PEMs require controlling of the adhesion behaviour by tuning their elastic/viscoelastic properties. In this study mechanical properties of LbL coated poly(L-lysine)/hyaluronan PLL/HA films were studied by scanning- and colloidal-probe atomic force microscopy as a function of indentation velocity, number of polymer deposition steps and temperature. Film growth was investigated by two independent AFM methods: scratch-and-scan and full-indentation[1]. Film thickness increases linearly with polymer deposition steps. The Young's modulus ranges between 15 and 40 kPa and does not depend on the film thickness. Stress relaxation and creep compliance measurements indicate a viscoelastic film behaviour with multiple relaxation mechanisms.

[1] ÜzüM, C.; Hellwig, J.; Madaboosi, N.; Volodkin, D.; v. Klitzing, R. *Beilstein J. Nanotechnol.* 2012, 3, 778*788.

CPP 13.3 Tue 10:15 H34

Single-Virus Force Measurements on sialic acid — ●VALENTIN REITER¹, SUMATI BHATIA³, MANUEL GENSLE¹, CHRISTIAN SIEBEN², DANIEL LAUSTER², ANDREAS HERRMANN², RAINER HAAG³, and JÜRGEN P. RABE¹ — ¹Department of Physics, Humboldt-Universität zu Berlin — ²Department of Biology, Humboldt-Universität zu Berlin — ³Department of Chemistry, Freie Universität Berlin

We study the multivalent effects in the binding and dissociation processes of sialic acid with the viral membrane protein hemagglutinin using scanning force microscopy (SFM) based single-virus force measurements (SVFM). Since an infectious disease has to start with the attachment of a virus to the cell membrane, this binding as well as its dissociation has to be carefully analyzed [1]. This is done by creating a mixed self assembled monolayer (MSAM) on gold from synthesized compounds, terminated by lipophilic acid. The compounds are functionalized with sialic acid and disfunctionalized with hydroxide. Inactivated influenza viruses are attached to a silicon nitrate SFM cantilever via a polyethylene glycol spacer. With this setup SVFM is performed

in aqueous solution. The ratio of functionalized to disfunctionalized molecules on the MSAM enables the control of the degree of multivalency of the binding and therefore the realization of mono-, bi-, and trivalent connections. On the other hand SVFM are performed at different loading rates to estimate specific binding parameters, such as the average rupture length and bond life time.

[1] C. Sieben et al., *PNAS*, 2012, 109, 34, 13626-13631.

CPP 13.4 Tue 10:30 H34

Response of major ampullate silk of *Nephila pilipes* to pressure and tensile stress as measured by FTIR spectroscopy — ●MARKUS ANTON¹, WILHELM KOSSACK¹, CHRISTOF GUTSCHE¹, ROXANA FIGULI², PERIKLIS PAPADOPOULOS³, and FRIEDRICH KREMER¹ — ¹Universität Leipzig, Institut für Experimental Physik I, Linnéstraße 5, 04103 Leipzig, Germany — ²Karlsruher Institut für Technologie, Institut für Technische Chemie und Polymerchemie, Engesserstraße 18, 76128 Karlsruhe, Germany — ³Max Planck Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany

Nanocrystals composed mainly of β -sheet polyalanine are responsible for the high toughness of major ampullate (dragline) spider silk. Fourier-Transform infrared (FTIR) spectroscopy is employed to study their response to (i) uniaxial stress and (ii) hydrostatic pressure. In the former a red shift and in the latter a blue shift of the vibration of polyalanine β -sheets at 965 cm^{-1} is observed. In both cases a linear dependence is evident, which bends off for hydrostatic pressure greater than 1.4 GPa and is fully reversible up to 7 GPa. The seamless connection of negative and positive pressure regimes corroborate quantitatively our structural model of spider silk [P. Papadopoulos et al., *Eur. Phys. J. E* 24 (2007) 193, P. Papadopoulos et al., *Colloid Polym. Sci.* 287 (2009) 231, R. Ene et al., *Soft Matter* 5 (2009) 4568] as composed of *pre-stressed* alanine-rich nanocrystals embedded in a glycine-rich amorphous matrix. It is also confirmed that nanocrystals withstand high pressures without undergoing structural transition or deteriorating their mechanical properties.

CPP 13.5 Tue 10:45 H34

Polarized confocal Raman microscopy and EBSD: A comparative study studying calcite crystalline regions within the tergite cuticle of terrestrial isopods. — ●CHRISTIAN REISECKER¹, ERIKA GRIESSHABER², BASTIAN SEIDL³, ANDREAS ZIEGLER³, and SABINE HILD¹ — ¹Institute of Polymer Science, Johannes Kepler Universität Linz, Altenbergstr. 69, 4040 Linz, Austria — ²Department of Earth and Environmental Sciences, LMU, Theresienstr. 41, 80333 München, Germany — ³Facility for Electron Microscopy, University of Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

Recently, isopods gained increasing amount of interest in terms of biomimetics as they combine quite diverse properties within their tergite cuticle such as hardness in the outer parts of the cuticle and softness in the more inner part, where muscles will be attached. This is achieved via a strong hierarchical arrangement of organic-chitin-protein fibers, which are arranged in a twisted plywood structure and inorganic materials. The organic matrix is hardened by carbonates in crystalline (calcite) and non-crystalline modification (amorphous calcium carbonate, ACC). This study focusses on the outer, mainly crystalline parts within the tergite cuticle of isopods. Confocal Raman microscopy is a useful tool to study the chemical and structural composition of isopods, as it provides a spatial resolution below 300 nm. Polarized confocal Raman microscopy and EBSD will be utilized to determine different domains and layers of calcite crystals. It has been demonstrated that depending on the species, the calcite region consists of domains with different orientations concerning its bravais lattice.

CPP 13.6 Tue 11:00 H34

Mineralization of calcium containing compounds at the liquid-liquid interface — ●STEFFEN BIEDER¹, FLORIAN WIELAND², PATRICK DEGEN³, MICHAEL PAULUS¹, JULIA NASE¹, ANDRE STEFFEN¹, BRIDGET MURPHY⁴, HEINZ REHAGE³, and METIN TOLAN¹ — ¹Fakultät Physik/DELTA, Technische Universität Dortmund, D-44221 Dortmund, — ²Helmholtz Zentrum Geesthacht, Max-Planck-Straße 1, D-21502 Geesthacht — ³Fakultät Chemie, Technische Uni-

versität, D-44221 Dortmund — ⁴Institut für Experimentelle und Angewandte Physik, CAU, Leibnizstraße 19, D-24098 Kiel

Nature forms structures from inorganic and organic components for different purposes, e.g. protection or stabilization. Accordingly, organisms have developed the concept of biomineralization providing highly controlled growth processes under ambient conditions. For instance the formation of teeth, bones or shells demonstrates the high degree of perfection and control, which can not be reached by human technology until now. We studied the mineralization of calcium containing compounds at the liquid-liquid interface. A solution of water and calciumhydrogencarbonat is covered by toluene. We added different fatty acids in order to investigate their influence on the growing layer at the liquid-liquid interface. We observed the layer formation by grazing incidence diffraction (GID) and x-ray reflectivity (XRR). The extracted data show an formation of calcium soaps at the interface. GID data reveal that the forming crystallites are highly orientated with the 001 axis perpendicular to the sample surface. We acknowledge BMBF(05 K10 FK2) and (05K10PEC) for financial support.

15 min. break

CPP 13.7 Tue 11:30 H34

Probing the electronic structure of Proline in aqueous solution by soft RIXS — ●FRANK MEYER¹, ANDREAS BENKERT^{1,2,8}, SANKARANARAYANAN NAGARAJAN³, REGAN WILKS⁴, MARCUS BÄR⁴, WANLI YANG⁵, MICHAEL ZHARNIKOV³, CLEMENS HESKE^{2,6,7}, LOTHAR WEINHARDT^{2,6,7}, and FRIEDRICH REINERT^{1,8} — ¹Exp. Phys. VII, Universität Würzburg — ²Inst. for Photon Science, KIT — ³Angew. Phys. Chemie, Universität Heidelberg — ⁴Solar Energy Research, HZB — ⁵ALS, Lawrence Berkeley National Laboratory — ⁶Dept. of Chemistry, University of Nevada, Las Vegas — ⁷ANKA Synchrotron Radiation Facility, KIT — ⁸Gemeinschaftslabor für Nanoanalytik, KIT

Amino acids are organic molecules that are highly relevant for many biological macro-molecules. Defining their function, the electronic structure of these molecules and, in particular, the interaction with biologically relevant solvents is of fundamental interest. In contrast to the majority of amino acids in which the functional groups (carboxyl, amino, side chain) are connected via one carbon atom, in proline the amino group and the side chain are connected in a heterocyclic compound, forming a pyrrolidine ring. We present resonant inelastic soft x-ray scattering (RIXS) maps of proline in aqueous solution at different pH values. Upon protonation and deprotonation, strong changes in the maps are observed. The results will be compared with RIXS data of solid state and gas phase proline, as well as other amino acids (i.e., glycine, cysteine). We find a distinctly different electronic structure than that observed for glycine and cysteine, as well as a significantly influence of the water environment.

CPP 13.8 Tue 11:45 H34

Structure formation in homologous peptides: Ac-Ala₆-Lys(H⁺) versus Ac-βAla₆-Lys(H⁺) — ●FRANZISKA SCHUBERT, CARSTEN BALDAUF, MARIANA ROSSI, VOLKER BLUM, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der MPG, Berlin

β-peptides are non-natural peptides composed of β-amino acid residues that feature one additional methylene group in the backbone compared to natural α-amino acids. Due to their larger flexibility, β-peptides are valuable for the design of new peptides with specific chemical or pharmacological properties. We here investigate the differences in structure formation between α- and β-peptides from first principles employing density-functional theory (DFT) with the PBE functional corrected for van der Waals interactions[1]. We focus this presentation on a comparison of Ac-βAla₆-Lys(H⁺) and Ac-Ala₆-Lys(H⁺) under *in vacuo* “clean-room” conditions and compare to experimental ion mobility spectrometry[2]. Our conformational search is based on replica exchange molecular dynamics. After generating a large pool of force field-based structures, we relax thousands of conformers with DFT. For the β-peptide, the finite-*T* vibrational free energy part is essential to recover a conformational hierarchy consistent with experiment. While Ac-Ala₆-Lys(H⁺) is found to be α-helical at 300K, Ac-βAla₆-Lys(H⁺) is seen to vary between 3₁₀, α, and π analog helices. Our simulations show that conformational entropy plays a critical role, and an *ab initio* quantitative assessment is a big challenge that we (and the field) must meet next. [1] A. Tkatchenko, M. Scheffler, PRL **102**, 073005 (2009); [2] S. Warnke, K. Pagel, G. von Helden, Fritz-Haber-Institut.

CPP 13.9 Tue 12:00 H34

Structure and Dynamics of Myelin Basic Protein as a Model System for Intrinsically Disordered Proteins — ●ANDREAS STADLER¹, LAURA STINGACIU², AUREL RADULESCU³, OLAF HOLDERER³, CLEMENT BLANCHET⁴, RALF BIEHL¹, and DIETER RICHTER¹ — ¹Forschungszentrum Jülich, JCNS-1/ICS-1, 52425 Jülich, Germany — ²Forschungszentrum Jülich, JCNS, Outstation at the Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — ³Forschungszentrum Jülich, JCNS, Outstation at FRM II, 85747 Garching, Germany — ⁴EMBL, Hamburg Unit, EMBL c/o DESY, Notkestrasse 85, Hamburg 22607, Germany

Myelin basic protein (MBP) is a major component of the myelin sheath in the central nervous system. In aqueous solution MBP is primarily unstructured. From a biophysical point of view, the disordered protein can serve as a model system to study the physical properties of disordered or unfolded proteins.

Neutron and X-ray scattering experiments were performed on the protein in solution. Small angle scattering and neutron spin-echo spectroscopy allowed us to gain quantitative information on the structural and the dynamical properties of MBP. The results of these experiments will be presented and compared to different models of polymer theory.

CPP 13.10 Tue 12:15 H34

Structure and disintegration of nanoparticles from clinically relevant polymers — ●MARGARITA DYAKONOVA¹, ANNA BOGOMOLOVA², SERGEY FILIPPOV², AUREL RADULESCU³, and CHRISTINE M. PAPADAKIS¹ — ¹TU München, Physik-Department, Physik weicher Materie, Garching — ²Institute of Macromolecular Chemistry, Prague, Czech Republic — ³JCNS at FRM II, Garching

We investigate clinically relevant polymers based on N-(2-hydroxypropyl methacrylamide) (HPMA) which carry both a cancer drug, namely doxorubicin, and a hydrophobic targeting group, namely cholesterol derivatives. We focus on the dependence of the structure of the nanoparticles formed by these conjugates on the polymer architecture, the cholesterol content of cholesterol and the pH value [1]. Fluorescence correlation spectroscopy showed that the onset of nanoparticle formation depends on the cholesterol content. A step-like increase of the hydrodynamic radius with conjugate concentration indicates that the existing nanoparticles associate rather than to grow continuously. SANS revealed that even small amounts of cholesterol derivatives results in the formation of nanoparticles. At neutral pH values, these are ellipsoids, whereas under acidic conditions, cholesterol is released and forms large crystals. Time-resolved SANS during a stopped-flow experiment showed that, in dependence of the hydrophobicity of the cholesterol derivatives, a change in pH leads to changes of the conformation of the HPMA chains.

[1] S. Filippov, M. Dyakonova, C.M. Papadakis et al., *Biomacromolecules* **13**, 2594 (2012)

CPP 13.11 Tue 12:30 H34

Reduction - oxidation photocycle dynamics of flavins in starch films — ●ALFONS PENZKOFER — Fakultät für Physik, Universität Regensburg, Universitätsstrasse 31, D-93053 Regensburg, Germany

The blue-light photo-reduction and dark re-oxidation of the flavins riboflavin and lumiflavin in starch (α-amylase) films was studied by absorption and luminescence spectroscopy. Blue-light sample excitation caused an absorption, fluorescence, and phosphorescence decrease which recovered in the dark. The photo-reduction and dark re-oxidation cycle could be repeated. The efficiency of photo-reduction decreased with exposed excitation energy, and the speed of re-oxidation in the dark slowed down with time after excitation. The absorption did not fully recover. The fluorescence efficiency after long time of storage in the dark increased beyond the initial oxidized flavin fluorescence efficiency. Flavin photo-excitation is thought to cause a starch-flavin restructuring (static fluorescence quenching center formation) enabling enhanced photo-induced starch to flavin electron transfer with subsequent flavin reduction and starch oxidation (oxystarch formation). In the dark after light switch-off, thermal reversion of flavin reduction and starch oxidation occurred and fluorescence quenching decreased.

CPP 13.12 Tue 12:45 H34

Study of phase transitions on DPPC bilayers deposited by PVD on top of low viscosity chitosan scaffolds of different thicknesses — ●MARIA J. RETAMAL, CARMEN GONZALEZ, MAURICIO SARABIA, MARCELO CISTERNAS, and ULRICH G. VOLKMANN — Surface Lab, Fac. de Física, P. Universidad Catolica de Chile, Chile

The porous nature of chitosan and its non-solubility in water could be an efficient matrix able to absorb water molecules and their delivery to a system. Chitosan of low viscosity (CH) and 1,2 *dipalmitoyl-sn-3-phosphoglycerocoline (DPPC) over silicon wafer (SiO₂/Si(100)) as substrate were used to conform an artificial membrane, silicon wafer/CH-DPPC. The deposition was made by Physical Vapor Deposition (PVD) and thickness was controlled in situ with Very High Resolution Ellipsometry (VHRE), achieving chitosan films with precise thicknesses between 10Å and 200Å, and a 60Å thin DPPC bilayer on top. We focus on the precise thickness control of the thin films, and

the related formation of interstitial channels, that favor the prolonged humidification in the system and the discovery of the most suitable thickness of the chitosan scaffold for best artificial membrane formation and stability. The characterization of the artificial membrane was realized using VHRE, IE (Imaging Ellipsometry) and Atomic Force Microscopy (AFM), with the finality to determine the possible phase transition temperatures.

M.J. R. and C. G. acknowledges CONICYT and VRI Nr. 10/2010 (PUC), respectively. Work supported by FONDECYT project Nr. 1100882.

CPP 14: Crystallization, Nucleation and Self Assembly I

Time: Tuesday 9:30–13:00

Location: H39

CPP 14.1 Tue 9:30 H39

Protein clustering as a precursor of crystallization — ●FAJUN ZHANG¹, ANDREA SAUTER¹, MARCELL WOLF¹, FELIX ROOSEN-RUNGE¹, MICHAEL SZTUCKI², ROLAND ROTH³, and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik, Universität Tübingen — ²ESRF, Grenoble, France — ³Institut für Theoretische Physik, Universität Tübingen

Protein clusters are normally considered as a major impurity for growth of high quality single crystals. Here we show that pre-assembled protein clusters formed via cation bridging can serve as a building block of crystallization. Globular proteins, human serum albumin and beta-lactoglobulin have been crystallized from solution in the presence of multivalent metal ions. These negatively charged globular proteins undergo a reentrant condensation phase behavior [1]. Crystallization near phase boundaries follows different mechanisms [2]. DLS and SAXS reveal the formation of protein clusters near both phase boundaries. Real time SAXS measurements demonstrate that protein clusters act as precursors of nucleation with a reduced energy barrier [3]. Crystallographic analysis provides direct evidence of the crystal structure and cation binding sites [2]. Although the binding sites do not necessarily form the crystal lattice, they enhance interactions between protein contacts. The limited binding number (2-4) ensures the flexibility of proteins within clusters, which is crucial for the conformation relaxation during nucleation. [1] F. Zhang, et al. Phys. Rev. Lett. 2008, 101, 148101. [2] F. Zhang, et al. J. Appl. Cryst. 2011, 44, 755. Soft Matter 2012,8, 1313. [3] F. Zhang, et al. Faraday Discuss. 2012, 159, 313.

CPP 14.2 Tue 9:45 H39

Structural evolution of a dense liquid phase in protein solutions — ●ANDREA SAUTER, FAJUN ZHANG, and FRANK SCHREIBER — Universität Tübingen, Institut für Angewandte Physik

Liquid-liquid phase separation (LLPS), the reversible transformation from a homogeneous into a protein rich and a protein poor phase, can be regarded as the equivalent of a gas-liquid transition. Here we present a study of the structural evolution of LLPS in solutions of beta-lactoglobulin (BLG) in presence of YCl₃. This system was subject of our research before [1,2] and has turned out to be a good model system for two-step crystallization. Selected samples were prepared at 35°C, above their critical temperature T_c of ca 20°C. When quenched to 5°C, the solution phase separates. Using SANS and SAXS, we followed the evolution of structures at different length scales. We use protein clusters based on the crystal structure to calculate theoretical scattering curves and compare them to the measured data. The results suggest the hierarchy of protein clusters to change with temperature and time. Comparison between initial and later measurements shows an increase at low q (clusters), at 1.8 nm⁻¹ (dimer formfactor) and several intermediate q regions and a simultaneous decrease in others. A decrease of the monomer-monomer correlation peak at 2.2 nm⁻¹ suggests the mobility of monomers within clusters to be changed in this process. The mobility of proteins within clusters and their relaxation are crucial for nucleation, so these findings will help the understanding of two-step crystallization. [1] F. Zhang et al., J. Appl. Cryst. 44, 2011, 755-762; [2] F. Zhang et al., Faraday Discuss. 159, 2012, 313-325.

CPP 14.3 Tue 10:00 H39

Entanglement Related Memory Effect in Primary Nucleation of Polymers — ●CHUANFU LUO¹ and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden, Germany —

²Technische Universität Dresden, Germany

Polymer crystallization is a non-equilibrium process and highly dependent on the thermal history. In self-seeding experiments a polymer melt is prepared by melting semi-crystalline polymer for a short time, followed by a subsequent cooling process, which can result in strong position and orientation- correlations of the resulting crystals with the previously crystalline regions [1-2]. The origin of such a memory effect is still unclear. We found indications that this memory effect is related to the state of entanglement in the melt which is still incompletely re-entangled during the heating period. By using MD simulations combined with primitive path analysis (PPA)[3], we reproduced self-seeding effects in simulations and we can show that crystallization and in particular self-seeding is directly correlated with the entanglement state of the melt. Also, we show that self-seeding takes place even for the case that all individual chains are in the molten state before cooling. [1]A. Mamun et al., Macromolecules 40, 6296-6303 (2007) [2]J.-J. Xu et al., Nature Mater. 8, 348 (2009) [3]R. Everaers et al., Science 303, 823-826 (2004)

CPP 14.4 Tue 10:15 H39

Effect of the Crystalline α_c -Process on the Morphology of Semicrystalline Polymers: a Comparative SAXS- Study on Poly- ϵ -Caprolactone and Polyethyleneoxide — ANNE SEIDLITZ, THOMAS THURN-ALBRECHT, ●RUTH BÄRENWALD, and KAY SAALWÄCHTER — MLU Halle-Wittenberg, 06120 Halle (Saale)

Semi-crystalline polymers can be classified into two different types, depending on the presence (α_c -mobile) or absence (crystal-fixed) of the α_c -relaxation, which provides mobility to the chains in the crystals. Starting from a hypothesis of Boyd, that all polymers with a high crystallinity are α_c -mobile while all polymers with a low crystallinity are crystal-fixed, we investigated the morphology of polyethyleneoxide as a polymer with mobile crystalline chains and poly- ϵ -caprolactone as a polymer with fixed chains. We performed small-angle X-ray scattering experiments and developed a simulation based on the paracrystalline model to derive quantitative morphological information from the SAXS data. Clear differences between the structure of PEO and PCL were observed. For PCL the crystalline thickness d_c is well defined, while the amorphous thickness d_a displays a broad distribution. PEO shows a small, well defined d_a and a broad thickness distribution of the crystalline lamellae. This confirms a different mode of structure formation. The crystalline lamellae in PEO, where thickening begins already at the growth front, can reorganize during crystallization until a minimal d_a , possibly reflecting a locally equilibrated entanglement structure, is established. For PCL no thickening of the initially formed lamellae is possible and the amorphous parts are randomly filled.

CPP 14.5 Tue 10:30 H39

10-nm structure formation induced by crystallization in P3HT/PCBM blends — ●ALESSANDRO SEPE¹, PETER KOHN¹, ZHUXIA RONG¹, KAI H. SCHERER¹, MICHAEL SOMMER², PETER MÜLLER-BUSCHBAUM³, RICHARD H. FRIEND¹, ULLRICH STEINER¹, and SVEN HÜTTNER¹ — ¹Cavendish Laboratory, University of Cambridge, Cambridge, UK — ²Institute of Macromolecular Chemistry, University of Freiburg, Freiburg, Germany — ³Lehrstuhl für Funktionelle Materialien, Physik-Department, TU München, Garching, Germany

Structural characterisation of novel semiconducting polymers is of great importance to the development of new materials for organic electronic applications. The solubility and aggregation of [6,6]-phenyl

C61butyric acid methyl ester (PCBM) within a polymer matrix is of great interest for the development of fullerene based organic photo-voltaic cells. Our study aims at methodically investigating the loading of a polymer with PCBM. For our investigation a specially synthesized mono-disperse regio-regular poly-(3-hexylthiophene-2,5-diyl) (P3HT) is used. The relative crystallinity of P3HT has been directly related to the nucleation density for PCBM aggregation. A combination of small, wide and grazing incident angle X-ray scattering techniques is used to track PCBM within the polycrystalline superstructure of P3HT. We have found the solubility limit of PCBM in amorphous P3HT domains, whereas, above this limit, it segregates out. Our results show that the crystallization of P3HT with crystal sizes in the range of 10 nm sets one of the length scales in the phase separation process.

CPP 14.6 Tue 10:45 H39

Heterogeneous Nucleation in Epitaxially Crystallized Polyethylene on Graphite — ●ANN-KRISTIN LÖHMANN, THOMAS HENZE, and THOMAS THURN-ALBRECHT — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Germany

We investigate the interface between a polymer melt and a crystalline substrate to get a more microscopic understanding of heterogeneous nucleation.

As a model system we studied crystallization and melting in thin epitaxially crystallized LLDPE films on graphite by high temperature AFM measurements. Upon heating above the melting temperature the polymer film starts to dewet and leaves a thin (only few nanometres) ordered film of polyethylene with a temperature dependent thickness behind. This ordered layer at the polymer-substrate interface shows the same lamellar structure as the semicrystalline film at lower temperatures. The thickness of the ordered layer and as a consequence the dewetting of molten polymer is reversible. The temperature dependence of the stabilized layer can be described by a phenomenological thermodynamic theory [1].

In this epitaxial system a stabilized ordered layer completely wets the substrate at temperatures above the bulk melting point and acts as a nucleus for crystallization, thus explaining the unusual lamellar structure of the crystalline film observable at room temperature.

[1] M. Heni and H. Löwen, *Phys. Rev. Lett.* **85**, 3668-3671 (2000)

CPP 14.7 Tue 11:00 H39

Real-time GISAXS-study of DIP thin film growth — ●CHRISTIAN FRANK¹, JIŘÍ NOVÁK¹, RUPAK BANERJEE¹, STEFAN KOWARIK², ALEXANDER GERLACH¹, and FRANK SCHREIBER¹ — ¹University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — ²Humboldt University of Berlin, Newtonstr. 15, 12489 Berlin, Germany

We present a real-time *in situ* grazing incidence small angle X-ray scattering (GISAXS) study on growth of diindenoperylene (DIP) [1] thin films on SiO_x substrates at various growth rates and substrate temperatures. DIP is a typical candidate for an active material in organic photo-voltaic and device applications. It is therefore important to understand how different growth parameters influence the evolution of the thin film morphology. By employing high brilliance synchrotron radiation and most recent CCD-area detectors we were able to monitor specular [2] and diffuse growth-oscillations simultaneously and in real-time. While the specular scattering contains information about crystallinity and morphology perpendicular to the sample surface, GISAXS data reflect also the lateral correlation lengths of surface features of thin films [3]. In this way we are able to monitor formation and coalescence of molecular islands during the layer-by-layer growth and the transition to the 3-D growth.

[1] A. C. Dürr et al., *Phys. Rev. Lett.* **90** (2003), 016104;
[2] S. Kowarik et al., *Eur. Phys. J. Special Topics* **167** (2009), 11;
[3] S. K. Sinha et al., *Phys. Rev. B* **38** (1988), 2297

15 min. break

CPP 14.8 Tue 11:30 H39

Melting Temperature and Crystal Growth Rate in Liquid Mixtures — ●KONSTANTIN KOSCHKE¹, DAVIDE DONADIO¹, HANS JÖRG LIMBACH², and KURT KREMER¹ — ¹MPI Polymer Research, Mainz, Germany — ²Nestlé Research Center, Lausanne, Switzerland

Crystallization of liquids is of uttermost interest for many disciplines, including materials, atmospheric and food science. The introduction of additives in solution allows the control of the key thermodynamics and kinetics parameters of crystallization, namely the transition tempera-

ture and the growth rate. Here we investigate the basic principles of crystallization of solutions by computing the melting temperature and simulating crystal growth of Lennard-Jones binary mixtures, by equilibrium and non-equilibrium molecular dynamics (EMD - NEMD) simulations. Both melting temperatures and growth rates are computed exploiting the two-phase method at equilibrium and non-equilibrium conditions, respectively. The effect of hydrophobic and hydrophilic solutes at low concentrations (< 3%) is analyzed, scanning systematically size and concentration. Our MD simulations allow us to connect macroscopic thermodynamic and kinetic observables, such as phase coexistence temperature and crystal growth rate, to the microscopic structure of the solutions and to microscopic processes occurring during crystal growth.

CPP 14.9 Tue 11:45 H39

Influence of Organic Ligands on ZnO Nanoparticle Formation via in-situ XRD — ●MIRIJAM ZOBEL — Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen

Organic ligands are used in solvent-based sol-gel processes to synthesize monodisperse, metal oxide nanoparticles for semiconductor industry. The ligand type and chemistry have a decisive influence not only on the particle size, but also on the structure and kinetics during the nucleation. Using high-energy synchrotron radiation, it is possible to study this nucleation in-situ via x-ray wide angle diffraction, even in salt solutions with very low concentration (30 mM). Our model system zinc oxide exhibits a precursor structure of the metal salt, which is stable for several hours and exists both without and in presence of additional ligands, e.g. dimethyl-L-tartrate or pentantrione. Addition of an alkali results in an instantaneous transformation into larger precursor structures, which - after a further ligand-specific ripening time - again spontaneously start to nucleate to approx. 2 nm nanoparticles. This final nucleation of the particles surprisingly takes several hours. Here we report for the first time that such an in-situ high-energy x-ray wide angle diffraction experiment with synchrotron radiation is possible and that it reveals the phase formation and the growth of nanoparticles within organic solvents. By deducing the pair distribution function and hence the structure of the different phases present, more profound structure analysis can subsequently be carried out.

CPP 14.10 Tue 12:00 H39

Real time and in-situ investigations of the nucleation and diffusion during the growth of the fullerene C₆₀ using X-ray scattering — ●SEBASTIAN BOMMEL^{1,2}, NICOLA KLEPPMANN³, CHRISTOPHER WEBER², HOLGER SPRANGER², JIRI NOVAK⁴, PETER SCHÄFER², STEPHAN V. ROTH¹, FRANK SCHREIBER⁴, SABINE H.L. KLAPP³, and STEFAN KOWARIK² — ¹Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — ²Institut für Physik, Humboldt-Universität Berlin, Berlin, Germany — ³Institut für Theoretische Physik, Technische Universität Berlin, Berlin — ⁴Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany

The surface morphology and the structural order during the growth of the popular organic semiconductor C₆₀ were studied with simultaneous real-time and in-situ measurements of Grazing Incidence Small-Angle X-ray Scattering (GISAXS) and anti-Bragg growth oscillations during organic molecular beam deposition. For the characterization of the morphology during the growth the island density was extracted from 2D GISAXS patterns. From this we find a dependency of the island density on thickness and also temperature, i.e. 150 islands/μm² for 313 K and 10 islands/μm² for 353 K in the beginning of growth. From the anti-Bragg growth oscillations high structural order and layer-by-layer growth during the growth of multilayer films were found. From a comparison of the nucleation and the growth oscillations with the analytic Trofimov rate equations model and KMC simulations the diffusion energy and the Ehrlich-Schwoebel barrier can be estimated to be 0.5 eV and 0.1 eV, respectively.

CPP 14.11 Tue 12:15 H39

Spin Casting of Dilute Solutions to Control Nucleation and Growth — ●STEFAN KARPITSCHKA, CONSTANS WEBER, and HANS RIEGLER — MPI für Kolloid- und Grenzflächenforschung, Potsdam, Germany

We analyze the spin casting of dilute (ideal) binary mixtures of non-volatile solutes in volatile solvents as a prototype for evaporation-controlled processes that are increasingly used to deposit specifically structured (sub)monolayers (evaporation-induced self-assembly). The first analytical description of the thinning of a volatile liquid film simultaneously subject to spinning and evaporation is presented. It

shows, that the duration of a spin casting process is linked to the process parameters via power laws. A diffusion-advection model leads analytically to the equation governing the spatio-temporal evolution of the internal film composition. Its solution reveals that the solute concentration enrichment, its gradient, and its time evolution are related to the process parameters via power laws. The physics behind the power laws is uncovered and discussed [1]. This reveals universal insights into the interplay between the control parameters and their impact on the spatio-temporal evolution of the film composition of diluted mixtures. It also offers palpable guidelines to better understand and control the spin casting of non-ideal solutions. Experiments are presented which support the theoretical findings.

[1] S. Karpitschka, C. Weber, H. Riegler, PRL (2012), in revision.

CPP 14.12 Tue 12:30 H39

Nucleation and Growth of Copper Phthalocyanine from Solution — ●FATEMEH GHANI and HANS RIEGLER — Max Planck Institute f. Colloid & Interfaces, Potsdam-Golm, Germany

Unsubstituted Metal-phthalocyanines (Pc) are excellent electron donating molecules for OSC. Usually organic solar cells with Pcs are produced by vapor deposition due to low solubility, although solution based deposition (like spin casting) is cheaper and offers more possibilities to control the structure of the film. It is necessary to find the appropriate solvents, assess the solution deposition techniques, such as

dip coating, and spin casting and understand the nucleation and growth process for aggregation/precipitation and to use this knowledge to produce nanostructures appropriate for OSC. We prepared thin films of CuPc from solution in ambient air. The parameters (e.g. solution concentration profile) governing nucleation and growth are calculated based on the spin casting theory of a binary mixture of a nonvolatile solute and evaporative solvent and inter-molecular interactions.

CPP 14.13 Tue 12:45 H39

Glass transition and recrystallization of alcohols in silica nanochannels — ●DANIEL RAU¹, ROLF PELSTER¹, TOMMY HOFMANN², DIRK WALLACHER³, and PATRICK HUBER⁴ — ¹FR 7.2 Experimentalphysik, Universität des Saarlandes — ²Helmholtz Zentrum Berlin, Inst Complex Magnet Mat, D-14109 Berlin, Germany — ³Helmholtz Zentrum Berlin, Dept Sample Environm, D-14109 Berlin, Germany — ⁴Hamburg Univ Technol, Inst Mat Phys & Technol, D-21073 Hamburg, Germany

We studied the molecular dynamics and glass transition of n-alcohol confined in electrochemical etched silica nanochannels using broadband dielectric spectroscopy and neutron scattering. In contrast to the bulk alcohol confined alcohol exhibits a glass transition upon slow cooling but partial recrystallization occurs upon heating. This behaviour reflects the different temperature dependences of nucleation and crystal growth.

CPP 15: Organic Electronics and Photovoltaics II (joint session DS/CPP/HL/O)

Time: Tuesday 9:30–12:45

Location: H32

CPP 15.1 Tue 9:30 H32

Influence of triplet excitons on the lifetime of polymer based organic light emitting diodes — ●OILI PEKKOLA, ANDREA GASSMANN, CHRISTIAN MELZER, and HEINZ VON SEGGERN — Electronic Materials Division, Institute of Materials Science, Technische Universität Darmstadt, Petersenstr. 23, 64287 Darmstadt, Germany

Despite the promising development of polymer based organic light emitting diodes (PLEDs), device lifetime and stability are still among the most critical issues. One of the lifetime-related factors investigated to a lesser extent is the influence of the high density of non-emissive triplet excitons which could be responsible for local heating or act as traps for charge carriers, leading to a degradation of the device.

This study utilizes PLEDs based on poly(p-phenylene vinylene) (PPV) derivatives to understand the influence of triplet excitons on the fatigue by increasing their amount in the PPV film. This increase is achieved by blending different concentrations of the triplet sensitizer platinum (II) octaethylporphyrine ketone (PtOEPK) into the PPV matrix in order to convert PPV singlet excitons to triplets. One observes that in PLEDs both the t_{50} and t_{90} lifetimes are drastically shortened in the presence of PtOEPK. To rule out a possible influence of the sole presence of PtOEPK on charge carrier transport, single carrier devices with different sensitizer contents were prepared. In these devices, no fatigue is observed regardless of the sensitizer concentration, suggesting that the decrease in the lifetimes of the bipolar diodes is indeed caused by the increased triplet population in the diodes with sensitized polymer films and not by the sensitizer additive as such.

CPP 15.2 Tue 9:45 H32

Homogeneity of thin ZnTPP-films on silicon measured with reflectance anisotropy spectroscopy and Raman spectroscopy — ●STEPHAN PETER KATE¹, SIMONA POP¹, JÖRG RAPPICH², and KARSTEN HINRICHS¹ — ¹Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Albert-Einstein Str. 9, Berlin, 12489 Germany — ²Helmholtz-Zentrum für Materials and Energy GmbH, Kekulestraße 5, Berlin, 12489, Germany

Organic devices for electronic applications are an important field of research. To improve the efficiency of those components, the analysis of structure and homogeneity of thin films is of crucial importance. In this study we demonstrate that Reflectance Anisotropy Spectroscopy (RAS) and Raman spectroscopy are useful to investigate the homogeneity of thin films of zinc-tetra-phenyl-porphyrin (ZnTPP) on silicon substrates. The RAS spectra of the thin films show an optical anisotropy in the visible spectral range. Analyzing the anisotropy, conclusions about the homogeneity of the thin films can be drawn. The vibrational modes of the molecules seen with resonant Raman

spectroscopy are sensitive to the film structure. A pyrrole-bending mode in the region of 1075 cm⁻¹ serves us as a marker for the film homogeneity. The RAS and Raman results are correlated with AFM measurements.

CPP 15.3 Tue 10:00 H32

Morphology evolution of diblock copolymer based ZnO nanostructures upon solvent vapor treatment — ●KUHUSARKAR, CHRISTOPH SCHAFFER, ANNA NAUMANN, DANIEL MOSEGUI GONZALEZ, and PETER MÜLLER-BUSCHBAUM — TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

Nanostructured inorganic metal oxides with tunable morphologies are desirable for optimizing many potential applications in the field of gas/chemical sensing, catalysis and energy storage. Zinc oxide (ZnO) is chosen in the present study owing to its outstanding optical and electrical properties. Different ZnO nanostructures are synthesized using a suitable diblock copolymer template via sol-gel chemistry. Zinc acetate dihydrate is used as the suitable commercial precursor for ZnO. There are several possibilities to tune the morphology as most of the diblock copolymers respond to the external fields such as temperature and solvent vapor. Hence, tetrahydrofuran solvent vapor treatment has been employed to the as-prepared thin films corresponding a grid-like morphology for different annealing times. Grazing incidence small angle X-ray scattering (GISAXS) has been performed to probe the structural order over the entire film volume. Evolution of the morphology has been followed by GISAXS studies as a function of different solvent treatment times. The annealed films are subsequently calcined at a higher temperature in order to understand the preservation of higher orders in the ZnO structure even after removal of the diblock copolymer.

CPP 15.4 Tue 10:15 H32

Correlation of morphology and electronic properties of MoO₃ doped CBP layers I: TEM and electrical properties — ●DANIELA DONHAUSER^{1,2}, LEVIN DIETERLE^{1,2}, PAUL HEIMEL^{3,2}, TOBIAS GLASER^{3,2}, MAYBRITT KÜHN^{4,2}, MUSTAPHA AL-HELWI^{5,2}, RASMUS R. SCHRÖDER⁶, ERIC MANKEL^{4,2}, MICHAEL KRÖGER^{1,2}, and WOLFGANG KOWALSKY^{1,2} — ¹Institut für Hochfrequenztechnik, TU Braunschweig, Braunschweig — ²InnovationLab GmbH, Heidelberg — ³Kirchhoff-Institut für Physik, Universität Heidelberg, Heidelberg — ⁴Institut für Materialwissenschaft, TU Darmstadt, Darmstadt — ⁵BASF SE, Ludwigshafen — ⁶CellNetworks, Universität Heidelberg

Since electrochemical doping can significantly improve the performance of organic devices, the understanding of the fundamental properties of doped thin films is crucial. For a variety of different material systems

a very low doping efficiency was observed, although from energetical considerations a very efficient charge transfer is expected. Using bright-field TEM and electron tomography we show for MoO₃-doped CBP ((4,4'-Bis(N-carbazolyl)-1,1'-biphenyl) thin films that this low doping efficiency is due to filament-like dopant agglomeration which can be controlled by changing the substrate temperature during the evaporation process [1]. The observed morphology is finally correlated with electrical properties like charge carrier density and mobility and depending on the dopant concentration an anisotropic charge transport is observed.

[1] Donhauser et al., *Adv. Funct. Mater.*, 2012, 10.1002/adfm.201202089

CPP 15.5 Tue 10:30 H32

Correlation of morphology and electronic properties of MoO₃-doped CBP layers II: IR spectroscopic study —

•TOBIAS GLASER^{1,5}, SEBASTIAN BECK^{1,5}, DANIELA DONHAUSER^{2,5}, MAYBRITT KÜHN^{3,5}, BERND LUNKENHEIMER^{4,5}, ANDREAS KÖHN^{4,5}, ERIC MANKEL^{3,5}, and ANNEMARIE PUCCI^{1,5} — ¹Universität Heidelberg, Kirchhoff-Institut für Physik — ²Technische Universität Braunschweig, Institut für Hochfrequenztechnik — ³Technische Universität Darmstadt, Fachbereich Materialwissenschaft, Fachgebiet Oberflächenforschung — ⁴Universität Mainz, Institut für Physikalische Chemie — ⁵InnovationLab GmbH, Heidelberg

In order to obtain a further understanding on the charge transfer process in p-type doping using transition metal oxides, we performed in-situ FTIR-spectroscopy on thin layers of 4,4'-Bis(N-carbazolyl)-1,1'-biphenyl (CBP) doped with MoO₃. In the doped layers, charge transfer complexes (CTCs) are formed, that exhibit a broad electronic excitation in the near IR region. These CTCs are located at the interface of the MoO₃ agglomerates and the organic matrix, inducing an interface dipole. The intensity of this electronic excitation in the spectra of layers with various doping concentrations indicates a linear increase of the agglomerates' surface area with MoO₃ concentration. The vibrational changes in the spectra of the doped layers indicate a charge transfer of Z=1e within the CTCs. By cooling the substrate during the deposition process, the agglomeration of the dopants can be suppressed.

Financial support by BMBF (project MESOMERIE) is gratefully acknowledged.

CPP 15.6 Tue 10:45 H32

Correlation of morphology and electronic properties of MoO₃-doped CBP layers III: XPS and UPS study —

•MAYBRITT KÜHN^{1,4}, ERIC MANKEL^{1,4}, DANIELA DONHAUSER^{2,4}, TOBIAS GLASER^{3,4}, THOMAS MAYER^{1,4}, and WOLFRAM JAEGERMANN^{1,4} — ¹Technische Universität Darmstadt, Fachgebiet Materialwissenschaft — ²Technische Universität Braunschweig, Institut für Hochfrequenztechnik — ³Universität Heidelberg, Kirchhoff-Institut für Physik — ⁴InnovationLab GmbH, Heidelberg

Electro-chemical doping is a prerequisite to improve efficiency and conductivity of organic OLED materials. Here the p-type doping behavior of MoO₃ is analyzed using photoelectron spectroscopy (XPS/UPS). The doped CBP layers were evaporated and analyzed under UHV conditions. Concerning the Fermi level shift three different regimes can be distinguished: At low doping concentrations (< 9 mol%) a rapid shift towards the HOMO level of CBP can be observed, becoming less strong and finally saturating at a maximum shift of 1 eV at a doping concentration of 45 mol%. The electron transfer from CBP to MoO₃ leads to the formation of reduced MoO₃. Determining the amount of these species we get information of the surface to volume ratio of the MoO₃ clusters in dependence of the doping concentration. Also here three different regimes can be distinguished. The morphology and Fermi level shift regimes will be correlated discussing the dopant morphology as shown in Talk I. Finally the amount of transferred charges is calculated regarding the reduced MoO₃ species and is compared with the number of cations determined by IR-spectroscopy (Talk II).

Coffee break (15 min)

CPP 15.7 Tue 11:15 H32

Organic semiconductor devices on fibre shaped structures for smart textile applications. —

•TOBIAS KÖNYVES-TOTH, ANDREA GASSMANN, and HEINZ VON SEGGERN — Electronic Materials Department, Institute of Materials Science, Technische Universität Darmstadt, Petersenstraße 23, 64287 Darmstadt, Germany

In the development of smart textiles already realized prototypes utilize

embedded LEDs, displays or interactive communication devices based on inorganic semiconductor technology. Yet, these wearable smart textiles are not always comfortable since inorganic devices are stiff and rigid. On the other hand, organic electronic devices can be realized on flexible substrates employing very thin active layers of only about 100 nm thickness. The aim of the present work is to process organic semiconductor based devices directly on fibre surfaces. This task is challenging as manufacturing related problems due to the cylindrical shape of the fibre substrates and their small diameter of about 200 nm have to be overcome. Here, we present our findings on functional OLEDs on fibre substrates. Also the choice of proper fibre materials, ways to acquire smooth fibre surfaces and the structuring and encapsulation of fibre-shaped devices will be discussed. Additionally, methods to characterize the functionality of the devices, like angle dependence emission, will be presented.

CPP 15.8 Tue 11:30 H32

Doping of organic semiconductors in case of dopant precipitation: the internal interface charge transfer doping model —

•THOMAS MAYER^{1,2}, ERIC MANKEL^{1,2}, CORINNA HEIN¹, and WOLFRAM JAEGERMANN^{1,2} — ¹Technische Universität Darmstadt, Institute of Materials Science, Surface Science Division — ²Innovation Lab Heidelberg

Doping of organic semiconductors is of paramount interest for device optimization as in addition to improved conductivity, engineering of space charge regions at interfaces e.g. of donor acceptor heterojunction solar cells is achieved. Photoemission data taken at the synchrotron BESSY on co-sublimed and bilayer films of prototypical organic semiconductors as CuPc and spiro-MeoTAD and prototypical p-type organic and inorganic dopants as TCNQ and WO₃ show similar electronic trends, which can be explained assuming phase separation of the dopants within the matrix material. For metal oxides the precipitation is directly observed using TEM. For the doping induced variations of the matrix Fermi level in such semiconductor-dopant composites we propose the internal interface charge transfer doping model. According to this model the doping limit can be predicted from pristine matrix and pristine dopant electronic band diagrams. The model also admits of deriving measures that can be taken to improve doping efficiency.

CPP 15.9 Tue 11:45 H32

Molecular orientation at heterojunctions for organic photovoltaics studied by NEXAFS —

•ANDREAS OPITZ¹, NORBERT KOCH¹, ULRICH HÖRMANN², WOLFGANG BRÜTTING², CHRISTOPHER LORCH³, ALEXANDER HINDERHOFER³, FRANK SCHREIBER³, and ELLEN MOONS⁴ — ¹Inst. f. Physik, Humboldt-Universität zu Berlin, Germany — ²Inst. of Physics, University of Augsburg, Germany — ³Inst. of Applied Physics, University of Tübingen, Germany — ⁴Dept. of Physics and Electrical Engineering, Karlstad University, Sweden

Organic/organic heterojunctions are widely used in organic photovoltaic cells. The morphology at the interface, where the charge carrier separation takes place, plays an important role. In this contribution the interfaces between sexithiophene (6T) as donor and the acceptor materials fullerene (C₆₀) and diindenoperylene (DIP) [1] were analysed by angle resolved near-edge X-ray absorption fine structure spectroscopy and the results were compared to X-ray scattering data.

Different orientations are observed for molecules in the bulk, at free surfaces and at buried interfaces. Here, the orientation at the free surfaces depends on the substrate temperature during deposition for 6T but not for DIP. Furthermore, the acceptor molecules influence the orientation of the underlying 6T molecules. An improved crystallization and pronounced upright standing of the molecules in the underlying 6T film was observed upon deposition of C₆₀. In contrast the deposition of DIP on top of 6T leads to an orientational relaxation of the 6T molecules to the bulk inclination angle.

[1] U. Hörmann et al., *phys. stat. sol. RRL* 5 (2011) 241.

CPP 15.10 Tue 12:00 H32

Electronic interface properties of PCBM using photoelectron spectroscopy —

•JULIA MAIBACH^{1,2}, ERIC MANKEL^{1,2}, THOMAS MAYER^{1,2}, and WOLFRAM JAEGERMANN^{1,2} — ¹Technische Universität Darmstadt, Fachbereich Materialwissenschaft — ²InnovationLab GmbH, Heidelberg

The electronic interface properties of wet processed organic materials are of current interest as many fabrication techniques for organic electronic devices are based on inks. Photoelectron spectroscopy (PES) has proven to be a powerful method to investigate the electronic structure at semiconductor contacts. Due to high surface sensitivity of

PES, the interface is generally prepared step by step in UHV. For films deposited from solution we integrated a newly developed ultrasonic nebulizer unit to the UHV cluster-tool of the analytic competence center at the InnovationLab, Heidelberg. Dilute solutions of Phenyl-C61-butyric acid methyl ester (PCBM) in Chlorobenzene were used to deposit the material on ozone and polymer treated ITO as well as on gold to investigate the contact behavior of PCBM. With the nebulizer method layer thicknesses in the range of 10-20 Å can be achieved while repeated exposure to the nebulae increased step by step the emission intensities of the PCBM. Furthermore drop-casting of thicker layers has been performed allowing in combination the thickness dependent determination of the electronic properties. In case of PCBM on ozone treated ITO the HOMO spectra shift 0.4 eV to higher binding energy with increasing thickness, indicating the formation of a space charge region in PCBM due to electron transfer from ozone treated ITO.

CPP 15.11 Tue 12:15 H32

Carbon Nanotubes and Organic Solar Cells — ●GERHARD LACKNER¹, RICHARD BOUCHER², VLADIMIR SHVARTSMANN¹, VIKTOR BEZUGLY², INGOLF ENDLER³, MARIO KRUG³, FRANK MEISSNER³, MARTIN MKANDAWIRE⁴, and DORU C. LUPASCU¹ — ¹Universität Duisburg-Essen, Essen, Germany — ²Technische Universität Dresden, Dresden, Germany — ³Fraunhofer-Institut für Keramische Technologien und Systeme IKTS, Dresden, Germany — ⁴Verschuren Centre for Sustainability in Energy and the Environment, Cape Breton University, Canada

Materials like carbon nanotubes (CNT) attracted much attention by researchers all around the world due to their exceptional electrical, mechanical and chemical properties. Especially single-walled carbon nanotubes (SW-CNT) offer great opportunities in the field of new electrical devices, for instance field effect transistors based on their semiconductor properties. CNT are also used in organic photovoltaics (OPV) as acceptor material, to enhance charge carrier transport within

organic layers or as transparent electrodes. The application of CNT as acceptor material and for charge carrier enhancement is the main topic of this work. Therefore, we studied the photovoltaic device performance of different material combinations of CNT, regio regular Poly(3-Hexylthiophen-2,5-diyl) (rr-P3HT), Phenyl-C61-butyric acid methyl ester (PCBM) and copper phthalocyanine (CuPc). Furthermore, different device architectures were investigated and compared with each other.

CPP 15.12 Tue 12:30 H32

n-channel percolation in a pentacene-C60 ambipolar organic thin film transistor — SIMON NOEVER, STEFAN FISCHER, and ●BERT NICKEL — Ludwig-Maximilians-Universität, Fakultät für Physik & CENS, München, D

We present [1] a well balanced ambipolar organic field effect transistor with high hole and electron saturation mobilities of 0.28 cm²/Vs and 0.18 cm²/Vs, respectively. The structure and morphology of the respective films are analyzed using AFM and GIXS methods. Furthermore, we track the formation of a pentacene-C60 heterojunction by in-situ measurements during deposition of C60. Upon percolation of the n-channel, the heterojunction charges, acting as an additional top gate for the hole conducting channel. The fact that the p-channel threshold does not shift before the n-channel develops highlights two interesting findings for bilayer ambipolar TFTs. Apparently, before the C60 film percolates, the fullerene islands are electronically floating and the charging of the interface is confined to the pentacene-C60 contact area. Secondly, the threshold voltage shift of the p-channel upon fullerene percolation implicates the generation of a second hole conducting channel at the pentacene top surface. The introduced method demonstrates a way to evaluate the electrostatic situation in operating organic heterojunction devices. [1] S. Noever, S. Fischer, B. Nickel, *Advanced Materials* (in press)

CPP 16: Interfaces and Thin Films II (joint session with DECHEMA and VDI)

The session is a joint session with ProcessNet "Grenzflächenbestimmte Systeme und Prozesse" of DECHEMA and VDI.

Organizers: Thomas Danner (BASF), Leo Nick (DECHEMA) and Regine v. Klitzing.

Time: Tuesday 9:30–13:00

Location: H40

Invited Talk

CPP 16.1 Tue 9:30 H40

Functional nanolayers made from colloidal building blocks — ●ANDREAS FERY — University Bayreuth, Physical Chemistry II and Bayreuth Center for Colloids and Interfaces, Universitaetsstr. 30, 95444 Bayreuth, Germany

Colloidal particles are attractive building blocks for forming functional nanolayers. Already at the single particle level, even multiple functionalities like optical functionality or stimulus sensitivity can be established. These functionalities can be easily integrated into nanolayers, as particle immobilization typically does not require sophisticated specific coupling chemistry, but in many cases, physisorption relying on unspecific interactions is sufficient. Finally, multi-layer formation and/or lateral patterning can unlock novel properties, which arise from synergistic functional, as well as local or long range coupling effects.

We illustrate this concept with examples from the area of stimulus responsive layers using microgel- or block-copolymer building blocks. The stimulus sensitivity of those can be used for controlling the interaction of cells with surfaces, allowing for novel concepts in switchable cell culture surfaces or anti-fouling. As well, we discuss how non lithographic patterning of metallic colloidal particles can be used for controlling plasmonic coupling effects, leading to applications in sensorics and plasmonics.

CPP 16.2 Tue 10:00 H40

Vapor treatment of diblock copolymer thin films with perpendicular lamellar structure — ●JIANQI ZHANG¹, ALESSANDRO SEPE², DORTHE POSSELT³, JAN PERLICH⁴, XUHU SHEN¹, DETLEF-M SMILGIES⁵, and CHRISTINE PAPADAKIS¹ — ¹TU München, Physikdepartment, Fachgebiet Physik weicher Materie, Garching, Germany — ²University of Cambridge, Department of Physics, UK — ³Roskilde University, IMFUFA, Denmark — ⁴HASYLAB at DESY, Hamburg, Germany — ⁵Cornell University, CHESS, Ithaca NY, USA

Solvent vapor treatment results in complex swelling kinetics in self-assembled thin films. We have investigated the structural changes of P(S-b-B) diblock copolymer thin films with perpendicular lamellar structure using in-situ, real-time grazing-incidence small-angle X-ray scattering. Cyclohexane (CHX), which is slightly selective for the PB block, was used to vapor-treat the films. For the as-prepared film, the image displays straight diffuse Bragg rods (DBRs), which indicate the perpendicular lamellar orientation. During vapor treatment, the DBRs bend inwards which we attribute to tilting of a fraction of the lamellae away from the purely perpendicular orientation. Upon subsequent drying, straight DBRs reappear, i.e. the perpendicular orientation is recovered. Additional narrow and elongated DBRs appear during the final stage of the drying process. This finding points to the protrusion of PS domains at the film surface because the PB domains dry more slowly.

CPP 16.3 Tue 10:15 H40

Internal structure and dynamics of microgel films at solid interfaces — ●STEFAN WELLET¹, YVONNE HERTLE², MARCEL RICHTER¹, PETER MÜLLER-BUSCHBAUM³, THOMAS HELLWEG², and REGINE VON KLITZING¹ — ¹Stranski Laboratorium, Inst.f. Chemie, TU Berlin, 10623 Berlin — ²Fakultät f. Chemie, Physikalische Chemie III, Universität Bielefeld, 33615 Bielefeld — ³Physikdepartment E13, TU München, 85747 Garching

The physico-chemical properties of stimuli-responsive polymers attract great interest in basic research and lead to a lively discussion of potential technical applications. A prominent example are microgel systems, which undergo a temperature induced phase transition corresponding to a discontinuous shrinking with increasing sample temperature. Microgel particles can be organized as ultra-thin films at solid surfaces, e.g. silicon single crystal surfaces. This leads to changes in the shrinking behaviour and the LCST. For example, the LCST is reduced

between 1°C and several °C with respect to the bulk phase. These findings raise the question how the interactions with the solid surface affect the internal structure and dynamics of the microgel particles. In a series of surface sensitive scattering experiments we addressed this question mainly focussing on the correlation length in the polymer network. Here, we present GISANS measurements investigating a microgel containing the monomer NIPAM, cross-linked with BIS (2 mol-% with respect to the mass of NIPAM). Additionally, first measurements addressing the internal dynamics in this system using neutron spin-echo spectroscopy under grazing incidence (GINSE) are discussed.

CPP 16.4 Tue 10:30 H40

Determination of the inner morphology of organic solar cells with grazing incidence small angle neutron scattering — MATTHIAS A. RUDERER¹, ROBERT MEIER¹, LIONEL PORCAR², ROBERT CUBITT², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany — ²Institut Laue Langevin (ILL), 6 Jules Horowitz, 38042 Grenoble, France

Organic photovoltaic devices based on conducting polymers are of increasing interest. The device efficiency of an organic solar cell is determined by the inner morphology of the active layer. However, such inner morphologies are not easily detectable by real space imaging methods such as electron microscopy. In contrast, grazing incidence small angle neutron scattering (GISANS) is a unique tool for the characterization of the active layer morphology, in particular for donor-acceptor systems with polymer donor and small molecule acceptor blends. The scattering length density contrast in such blends is typically large, which makes special deuteration dispensable and real systems can be studied. For the example of P3HT:PCBM bulk heterojunction thin films the inner morphology is determined with GISANS. The phase separation structure and the amount of molecular intermixing are investigated as a function of the overall PCBM content. For the symmetric P3HT:PCBM ratio, which is typically highly efficient in photovoltaic devices, a structure size in the range of the exciton diffusion length, the largest PCBM phases and 18 vol% dispersed PCBM in the amorphous P3HT phase are found.

CPP 16.5 Tue 10:45 H40

Investigation of structure and molecular nature of the conjugated polymer films by hard and soft x-ray reflectivity and XAFS in reflection mode — ARMAN DAVTYAN, SOUREN GRIGORIAN, DMITRY KSENZOV, and ULLRICH PIETSCH — University of Siegen, Siegen, Germany

Structural and optical properties of the conjugated polymers were measured close and outside the K-absorption edge of carbon. Hard and soft x-ray reflectivity measurements are characterizing samples made of P3AT (poly(3-alkylthiophene)) thin films covered onto SiO₂ coated silicon substrates. The general structures of films were determined by combined fitting of hard and soft x-ray reflectivity curves. Additional chemical information was taken from the shape of curves taken by ReflEXAFS in the energy range of the Carbon K-edge (275-340 eV). It turns out that structural properties depend on the preparation technique used. Considering all information a three-layer model was appropriate to simulate the hard and soft x-ray reflection curves and the C K-edge ReflEXAFS profiles of the spin coated thin films.

CPP 16.6 Tue 11:00 H40

Hierarchical multiscale modelling of polymer-solid interfaces — KAREN JOHNSTON¹ and VAGELIS HARMANDARIS² — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²Department of Applied Mathematics, University of Crete, Greece

Polystyrene films sandwiched between two parallel gold surfaces were studied using hierarchical multiscale modelling. Classical all-atom polymer-surface interface potentials were developed based on density functional theory calculations that account for van der Waals forces [1]. All-atom molecular dynamics simulations were then used to study the structure and dynamics of 10mer polystyrene thin films up to 10 nm thick [2]. To study longer chains and thicker films a coarse-grained model was used [3] and the coarse-grained surface potentials were developed based on all-atom potential of mean force calculations. The results of the coarse-grained and all-atom simulations were compared for a 5 nm film of 10mer polystyrene and the results were in good agreement. The coarse-grained model was used to simulate 10 and 20 nm films for chain lengths of up to 200mer and the dependence of the structure, dynamics and interphase width on chain length were investigated.

- [1] Johnston and Harmandaris, J. Phys. Chem. C 115, 14707 (2011)
- [2] Johnston and Harmandaris, Soft Matter, 8, 6320 (2012)
- [3] Fritz et al. Macromolecules, 42, 7579 (2009)

15 min. break

CPP 16.7 Tue 11:30 H40

Relaxation of non-equilibrium entanglement networks in thin polymer films — PAUL D. FOWLER, JOSHUA D. MCGRAW, MELISSA L. FERRARI, and KARI DALNOKI-VERESS — Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada

It is well established that polymer films, prepared by spincoating, inherit non-equilibrium chain conformations which can affect macroscopic film properties. Here we present the results of crazing measurements [1] that elucidate the non-equilibrium chain configurations in spin-cast films. Furthermore, we find that the entanglement network equilibrates on a time scale comparable to one reptation time. In a second set of experiments, we confine polymers to films with thickness comparable to the molecular size. By stacking two such films at room temperature, a glassy bilayer film with a buried entropic interface is created. According to Silberberg's reflection principle, such an interface has an entropic cost associated with the restricted configurations of molecules that cannot cross the mid-plane of the bilayer. In the melt, the interface heals as chains from the two layers mix and entangle with one another. Crazing measurements reveal that it takes less than one bulk reptation time for a bilayer to become indistinguishable from a single film.

- [1] McGraw et al., EPJE (2012 - submitted).

CPP 16.8 Tue 11:45 H40

Nano-scale Roughness of Phase Boundaries in Heterogeneous Polymers: The rigid-mobile Interphase — MATTHIAS ROOS and KAY SAALWÄCHTER — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Germany

Many macroscopic features of polymers rely on microscopic and nano-scale characteristics, so their morphology, in particular nano-scale dynamic heterogeneities, is of great importance. Based on the possible distinction of differently mobile parts of the sample by proton NMR, we use an effect called spin diffusion (i.e. transport of spin magnetization among the nuclei) to investigate neighborhood relations between rigid and mobile (below or above T_g, respectively) components in semi-crystalline polymers and block copolymers. In addition, a phase of intermediate mobility can be identified.

If there is a selective magnetization of the rigid phase, first the magnetization induced signal of the interphase rises, followed by the magnetization of the mobile phase. That is to say, the magnetization diffuses from the rigid phase to the mobile one but must cross the respective interphase. Contrary to this, if a selective magnetization of the mobile phase is created, the rigid phase will gain its magnetization simultaneously with the interphase.

It was possible to replicate this effect by simulating the diffusive behavior of magnetization when taking into account a thickness variation of the rigid phase, where the interphase is mainly situated in "depressions" of the rigid phase, i.e., in regions that are less exposed to the mobile phase.

CPP 16.9 Tue 12:00 H40

Glassy dynamics of densely packed semi-isolated polymer chains — MARTIN TRESS, EMMANUEL MAPESA, and FRIEDRICH KREMER — Universität Leipzig, Leipzig, Germany

The glassy dynamics of randomly distributed, densely packed semi-isolated poly(2-vinylpyridine) (P2VP) polymer chains is studied by means of Broadband Dielectric Spectroscopy (BDS). Therefore, a recently developed nano-structured electrode arrangement is refined to achieve an electrode-to-electrode distance of only 40 nm. On one of the ultra-flat, highly conductive silicon electrodes semi-isolated polymer coils are deposited. Atomic Force Microscopy scans of the identical sample before and after the BDS measurement reveal that, even for different molecular weights, the mean volume of the coils resembles 5 to 10 times the volume expected for a single chain. Accordingly, the dynamics of coils on average consisting of 5 to 10 (therefore semi-isolated) polymer chains is measured and it compares well with that of bulk though the mean relaxation rate is slowed down by up to half a decade. This is attributed to attractive interactions of the P2VP segments with the supporting silica surface.

CPP 16.10 Tue 12:15 H40

Electric polarization in thin films of polyvinylidene fluoride doped with the ionic liquid 1-ethyl-3-methylimidazolium nitrate — ●ALEXANDER LACK, PETER FRÜBING, FEIPENG WANG, and REIMUND GERHARD — Applied Condensed-Matter Physics Group, Department of Physics and Astronomy, Faculty of Science, University of Potsdam, Karl-Liebknecht-Strasse 24-25, 14476 Potsdam, Germany

Dielectric properties of spin-coated polyvinylidene fluoride (PVDF) films containing a small amount (0.01 - 10 wt%) of the ionic liquid (IL) 1-ethyl-3-methylimidazolium nitrate [EMIM⁺][NO₃⁻] and sandwiched between aluminium electrodes are investigated. Films with more than about 1 wt% IL exhibit pronounced current-voltage hysteresis which indicates the existence of a ferroelectric polarization. The dielectric spectra show pronounced charge-carrier polarizations with huge permittivities. In films with more than 0.1 wt% IL electrode polarization dominates. From its signatures the DC conductivity is estimated: for films with 1 wt% IL values of 10⁻⁷ and 10⁻⁴ S/cm are found at room temperature and 100 °C, respectively. The relaxation associated with the glass transition in PVDF tends to disappear for samples containing more than 1 wt% IL, though the crystallinity is only moderately enhanced. These findings refer to an ordered crystalline structure where ions are immobilized by Coulomb interaction with molecular dipoles within the polymer chain. The details of this interaction have still to be understood.

CPP 16.11 Tue 12:30 H40

Segmental and chain dynamics in thin layers of poly(cis-1,4-isoprene) — ●EMMANUEL URANDU MAPESA¹, MARTIN TRESS¹, MANFRED REICHE², and FRIEDRICH KREMER¹ — ¹University of Leipzig, Linnestraße 5, 04103 Leipzig, Germany. — ²Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle an der Saale, Germany.

Broadband Dielectric Spectroscopy (BDS) - in combination with a nanostructured electrode arrangement - is used to study thin layers of poly(cis-1,4-isoprene) (PIP). Being a Type A polymer, PIP enables the investigation of two distinct relaxation modes taking place at two different length scales: the segmental motion which involves structures

of about one nanometer in size and the normal mode which represents the global dynamics of the chain. For molecular weights ($M_w = 24.5, 44.5, 53$ and 75 kg/mol) much greater than M_c (the critical molecular weight, $M_c = 10e+04$), down to thicknesses comparable to the respective radii of gyration, it is observed that: (i) the segmental mode as a local relaxation process is unaltered by the confinement in thin layers; (ii) the normal mode becomes faster with decreasing layer thickness, and (iii) this change in the normal mode is molecular-weight dependent. For M_w approximately equal to M_c , both the segmental and normal modes remain unaffected by changes in layer thickness.

CPP 16.12 Tue 12:45 H40

Azo-propellers as nanoscopic actuators in light-induced deformation of azobenzene polymer films — ●MARINA SAPHIANNIKOVA¹, VLADIMIR TOSHCHÉVNIKOV¹, and JAROSLAV ILNYTSKYI² — ¹Leibniz-Institut für Polymerforschung Dresden e.V. — ²Institute for Condensed Matter Physics, Lviv, Ukraine

We present the theoretical and MD simulation studies of thin azobenzene polymer films based on side-chain azo-oligomers having a stiff backbone and short spacers. Up to the glass transition temperature T_g the polymer backbone can be considered as a rigid prolate ellipsoid with a number of azobenzenes attached to it. Polar and azimuthal distributions of chromophores were studied at different temperatures and laser intensities. Their analysis was done in terms of nematic order parameters calculated in respect to the backbone. These parameters served then as input into a theoretical expression for the striction stress [1], which was found to be positive and above the yield stress. This explains irreversible elongation of the illuminated thin films below T_g , as found previously in experiment and MD simulations [2].

The light-induced reorientation of typical propeller-like structures is shown to be a microscopic reason of the sample elongation. Thus, molecular azo-propellers work as nanoscopic actuators which convert the light energy into material deformation. This finding opens a way for prediction of photomechanical properties of glassy azo-compounds directly from their chemical structure.

- [1] V.Toshchevnikov et al., J. Phys. Chem. B 113, 5032 (2009).
[2] J. Inytskyi et al., J. Chem. Phys. 135, 044901 (2011).

CPP 17: Glasses II (joint session DY/DF/CPP)

Time: Tuesday 9:30–12:30

Location: H46

CPP 17.1 Tue 9:30 H46

Towards reliable structural information of multicomponent glass systems — ●CHRISTOPH SCHERER^{1,2}, FRIEDRIKE SCHMID¹, and MARTIN LETZ² — ¹Johannes Gutenberg-Universität, Mainz, Deutschland — ²Schott AG, Mainz, Deutschland

Glasses have a huge range of applications, however, they are still theoretically not well understood. Also experimental access to the structure of glasses is limited. This motivates the study of glass systems by means of computer simulations.

In this work, a set of glass structures is generated on the computer by equilibrating a system of a few hundred atoms at high temperature, well above the glass transition temperature, with a classical molecular dynamics simulation (MD). Afterwards the system is cooled down to 0 K and structurally relaxed to the next (local) minimum by means of a quantum mechanical density functional (DFT) calculation. The glass properties before and after the structural relaxation are compared to experimental results. Especially, the phonon density of states is of interest, as it provides access to thermodynamical quantities.

This sets the basis for the next steps: The force fields for the MD simulation are generated by means of a structural fitting procedure. Here, the force field parameters are fitted in a way that the structure, namely the radial distribution function, of a short MD run at high temperature matches as closely as possible that one of a short DFT run at the same temperature. The dependence of the fitting accuracy of the classical force field on the final glass structure and glass properties is examined.

CPP 17.2 Tue 9:45 H46

On the behavior of supercooled liquid water in confinements formed by frozen water molecules: a molecular dynamics simulation study — ●FELIX KLAMETH and MICHAEL VOGEL — Institut für Festkörperphysik, TU Darmstadt, 64289 Darmstadt

Molecular dynamics simulations are performed to study the influence of an amorphous ice confinement on liquid water. Investigating water in confinement is believed to reveal information unaccessible for bulk water due to crystallization. Therefore, there are numerous studies on confined water, which claim, e.g., existence of a second critical point associated with a liquid-liquid phase transition in the supercooled regime [1]. However, transfer of information from confined water to bulk water is not straightforward because introducing walls changes the static properties of water due to specific interactions at the interfaces. To avoid this drawback, we use a neutral confinement comprised of immobilized water molecules. We compare static and dynamical properties found in pores with different radii to that of bulk water. The static characteristics, like the tetragonal order parameter, are not changed even near the pore wall. On the contrary, the dynamics inside the pore are dramatically influenced. We find a tremendous increase of the structural relaxation time of liquid water when approaching the pore wall. Thus, we observe a strong change of the local dynamics, which is neither accompanied by a variation of the local structure nor caused by specific wall-liquid interactions. Possible origins for this effect are discussed. [1] P. Kumar et al, PRL (2006), 97, 177802

CPP 17.3 Tue 10:00 H46

Deuteron-NMR investigation on the dynamics of supercooled, confined water — ●MATTHIAS SATTIG and MICHAEL VOGEL — TU Darmstadt, Institut für Festkörperphysik

The dynamical behaviour of water in the regime of the supercooled liquid is a topic of large interest. In particular, the existence of a fragile-to-strong transition (FST) at $T=225$ K related to the transition between two distinct phases of liquid water is controversially discussed [1]. Due to crystallization the temperature range proposed for the FST is hardly accessible in bulk water. Therefore, we confine heavy water to narrow pores in the mesoporous silicate MCM-41. This suppresses

the freezing of a substantial fraction of water, enabling direct investigation of the interesting temperatures. Deuteron-NMR methods are utilised to determine the rotational correlation times τ of water on time scales from ns up to s. The spin-lattice-relaxation time T_1 exhibits a typical minimum at about $T=230\text{K}$. Above this minimum the correlation times follow a Vogel-Fulcher-Tammann law. Below the minimum, two relaxation processes could be observed. The low-temperature processes show a different temperature dependence, where the curves $\tau(T)$ of all processes intersect at about $T=230\text{K}$. A comparison with literature data [2] from neutron scattering and dielectric spectroscopy gives rise to the idea that the observed crossover is due to this intersection of processes rather than to a FST. To test this idea studies on water confined to MCM-41 with different pore sizes and fillings are in progress.

[1] Mishima; Nature, Vol. 396, 329(1998) [2] Hedström; EPJST 141, 53(2007)

CPP 17.4 Tue 10:15 H46

Modelling the relaxation of glass-forming systems at low temperatures: a potential energy approach — ●ANDREAS HEUER and CHRISTIAN REHWALD — Institute for Physical Chemistry, Corrensstr. 28/30, D-48149 Münster

Based on finite-size effects of a model glass-forming system we have introduced a model which allows one to express the dynamics of a macroscopic glass-former in terms of coupled subunits of temperature-independent size and temperature-dependent coupling constant [1]. The results are obtained from computer simulations on a binary mixture Lennard-Jones model, interpreted in terms of the underlying potential energy landscape. The model is denoted coupled landscape model (CLM).

After a short review of the CLM we present key predictions of this approach for temperatures far below the range accessible by computer simulations. In particular we present results for the violation of the Stokes-Einstein relation (connecting diffusivity and structural relaxation) and the validity of the time-temperature superposition. Finally, the CLM is compared with other models presently discussed for the explanation of the glass-transition phenomena.

[1] C. Rehwald, O. Rubner, A. Heuer, Phys. Rev. Lett. 105, 117801 (2010)

[2] C. Rehwald, A. Heuer, Phys. Rev. E 86, 051504 (2012)

CPP 17.5 Tue 10:30 H46

Microrheology on supercooled liquids in terms of a Potential Energy Landscape approach — ●CARSTEN FRIEDRICH ERICH SCHROER and ANDREAS HEUER — Westfälische Wilhelms-Universität Münster, Münster, Germany

We perform MD simulations of a binary Lennard-Jones mixture where an external force is applied on a single tracer particle. The dynamics of the tracer particle includes several interesting features like non-linear mobilities and anomalous diffusion parallel to the force direction. Our main focus relies in the investigation of the underlying Potential Energy Landscape (PEL), especially in the energetic minima the system explores during its time evolution. Equally to equilibrium systems a coarse graining of these minima to mesoscopic regions allows the description of the system dynamics in terms of a continuous time random walk (CTRW). Extending the concept of the CTRW towards stationary non-equilibrium systems turns out to be an efficient tool for the understanding of non-equilibrium dynamics. First, the approach contains a decomposition between linear and non-linear effects, thus enables a detailed study of the transition between these dynamical regimes. Second, it allows the quantitative understanding of the anomalous diffusion of the tracer particle. Third, for the first time a connection between the non-Gaussian parameter α_2 in equilibrium and superdiffusivity in non-equilibrium can be established. With the help of the underlying PEL, important information can be gained about the dynamics, e.g. about the onset of non-linear effects. The non-linear regime can be discussed in terms of a rejuvenation scenario.

15 min. break.

CPP 17.6 Tue 11:00 H46

Simulation of Aging in SiO₂: Single Particle Jump Analysis — ●KATHARINA VOLLMAYR-LEE¹, ROBIN BJORKQUIST², and LONDON CHAMBERS³ — ¹Bucknell University, USA — ²Cornell University, USA — ³Texas A&M, USA

Using molecular dynamics computer simulations, we study the aging

dynamics of amorphous SiO₂. Starting from fully equilibrated configurations at high temperatures the system is quenched to temperatures which are below T_c . We then observe the resulting microscopic dynamics as a function of the waiting time t_w , the time elapsed since the temperature quench. We use single particle trajectories to identify "jumps" when the particle's average position changes over a short time interval significantly compared to its fluctuations. We find that the only tw-dependent microscopic quantity is the number of jumping particles per unit time. Similar to previous studies for fragile glass formers, we show here for the strong glass former SiO₂ that neither the distribution of jump lengths nor the distribution of times spent in the cage are tw-dependent. We therefore find a surprising similarity of the jump dynamics of fragile and strong glass formers.

CPP 17.7 Tue 11:15 H46

Excess free energy of supercooled liquids at disordered walls — ●RONALD BENJAMIN and JÜRGEN HORBACH — Institut für Theoretische Physik II - Soft Matter, Heinrich-Heine-Universität Düsseldorf

We perform NVT molecular dynamics simulations of a supercooled liquid confined between identical walls of two types. In the first case flat structureless walls, represented by an external field are considered. In the second case we consider disordered walls consisting of the same supercooled liquid frozen into an amorphous configuration. Using a thermodynamic integration scheme [R.Benjamin and J. Horbach, J. Chem. Phys. **137**, 044707 (2012)] we are able to obtain the excess free energy of the supercooled liquid with respect to both kinds of walls. While a positive excess free energy (of the order of $10k_B T/\sigma^2$) is obtained with respect to a flat structureless wall, the excess free energy between the supercooled liquid and the frozen disordered walls turns out to be negative ($\approx -0.5k_B T/\sigma^2$) even though the potential energy of the supercooled liquid in presence of the disordered walls is the same as that of the bulk. This shows the purely entropic contribution to the excess free energy of the supercooled liquid in presence of the disordered walls. The existence of a negative excess free energy also shows that the thermodynamic properties of such a confined supercooled liquid is not identical to that of the bulk.

CPP 17.8 Tue 11:30 H46

Multiple reentrant glass transitions of soft spheres at high densities — ●MICHAEL SCHMIEDEBERG — Institut für Theoretische Physik 2: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40204 Düsseldorf, Germany

We study the dynamics of soft spheres by using Molecular Dynamics simulations. The relaxation time varies non-monotonically as a function of density at constant temperature (cf. [1,2]). We determine and study the jamming phase diagrams that indeed show multiple reentrant glass transitions if temperature and density are used as control parameters. However, if we switch to a new formulation of the jamming phase diagrams [3], where temperature over pressure and pressure are employed as control parameters, no non-monotonic behavior can be observed.

[1] L. Berthier, A.J. Moreno, and G. Szamel, Phys. Rev. E 82, 060501(R) (2010).

[2] M. Pica Ciamarra and P. Sollich, arXiv:1209.3334.

[3] T.K. Haxton, M. Schmiedeberg, and A.J. Liu, Phys. Rev. E 83, 031503 (2011).

CPP 17.9 Tue 11:45 H46

Exact Nonlinear Response in the driven lattice Lorentz gas — ●SEBASTIAN LEITMANN and THOMAS FRANOSCH — Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058, Erlangen, Germany

We determine the nonlinear time-dependent response of a tracer on a lattice with randomly distributed hard obstacles as a force is switched on. The calculation is exact to first order in the obstacle density and holds for arbitrarily large forces. In particular, we show that the non-linear mobility in the stationary state becomes non-analytic in the driving force. Furthermore we demonstrate that the stationary velocity is approached exponentially fast for any finite values of the force, in striking contrast to the power-law relaxation predicted within linear response. We discuss the range of validity of our analytic results by comparison to Monte Carlo simulations.

CPP 17.10 Tue 12:00 H46

From beta-relaxation to alpha-decay: Atomistic picture from molecular dynamics simulations for glass-forming Ni_{0.5}Zr_{0.5} melt — ●HELMAR TEICHLER — Inst. Materialphysik, Univ Göttingen

In glass-forming melts the decay of structural fluctuation shows the well known transition from beta-relaxation (von-Schweidler law with exponent b) to alpha-decay (KWW law with exponent β). Here we present results from molecular dynamics simulations for a metallic glass forming Ni_{0.5}Zr_{0.5} model aimed at giving an understanding of this transition on the atomistic scale. At the considered temperature below mode coupling T_c , the dynamics of the system can be interpreted by residence of the particles in their neighbour cages and escape from the cages as rare processes. Our analysis yields that the fraction of residing particles is characterized by a hierarchical law in time, with von-Schweidler b explicitly related to the exponent of this law. In the alpha-decay regime the stretching exponent reflects, in addition, floating of the cages due to strain effects of escaped particles. Accordingly, the change from beta-relaxation to alpha-decay indicates the transition from low to large fraction of escaped particles.

CPP 17.11 Tue 12:15 H46

Interaction between tunnelling systems in glasses — ●GUDRUN FICKENSCHER¹, CHRISTIAN SCHÖTZ¹, PAUL FASSL¹, ALEXANDER ARCHER¹, ALEXANDER BURIN², MANFRED VON SCHICKFUS¹, ANDREAS FLEISCHMANN¹, and CHRISTIAN ENSS¹ — ¹Kirchhoff-Institut

für Physik, Universität Heidelberg — ²Tulane University, New Orleans, USA

The low-temperature properties of glasses are governed by tunnelling systems as described in the well-established standard tunnelling model. Interactions between tunnelling systems and phonons lead to energy relaxation. In addition, the interaction between individual tunnelling systems, as predicted by spectral diffusion theory, causes phase decoherence phenomena. To study these interaction processes we have measured the decay of different types of polarization echoes in the standard glass BK7 with respect to the delay time at temperatures between 7.5mK and 70mK. The decay of 2- and 3-pulse echoes is strongly influenced by spectral diffusion. In the case of 3-pulse echoes we expect, in addition, a significant contribution to the decay by energy relaxation processes. On comparing the measured data to numerical calculations we find that the decay of the echo amplitude is slower than predicted by the standard theory at all temperatures. This leads us to the assumption, that there exists a small subspace of tunnelling systems which interact very little with phonons due to a very small coupling constant. Including this subspace in the calculations we can accurately fit the data for all echo types and temperatures with one consistent set of parameters.

CPP 18: Poster: Polymer Dynamics

Time: Tuesday 18:15–20:15

Location: Poster C

CPP 18.1 Tue 18:15 Poster C

Transport of Polyelectrolytes in Rotational and Pulsed-DC Electric Fields in Confining Cylindrical Geometries — SORIN NEDELICU¹ and ●JENS-UWE SOMMER^{1,2} — ¹Leibniz Institute of Polymer Research Dresden e.V., Hohe Strasse 6, D-01069 Dresden, Germany — ²Technische Universität Dresden, Institute of Theoretical Physics, Zellescher Weg 17, D-01069 Dresden, Germany

We consider molecular dynamics simulations of the electrophoretic motion of charged polymers in a confining straight cylinder under the influence of an electric field which has a time-independent component orientated along the axis of the cylinder and a component perpendicular to the symmetry axis which rotates with constant angular velocity. The fluid is modeled explicitly, and also the co-ions, counterions and the charged polymer monomers. At moderate applied electric field in the axial direction, and nearly complete separation of the positive from the negative free charges, the electrophoretic velocities of the charged polymer chains in a narrow window of rotational frequencies are found to depend strongly on hydrodynamic friction effects related to changes in the frontal cross-section area and extension due to axial and centrifugal forces. We also investigate electrophoresis in cylinders with a periodic variation (or modulation) of the diameter. In these modulated geometries, the charged polymer chains can be separated only at low fields. At large fields we observe separation effects in modulated geometries if a pulsed electric field is applied. We propose scaling arguments to explain the observed behavior.

CPP 18.2 Tue 18:15 Poster C

Behavior of AB-Diblock-Copolymer chains under the influence of external Stimuli - An AFM Study — ●KIRSTEN DAMMERTZ, ANNE-MARIE SAIER, MASOUD AMIRKHANI, MARTIN MUELLER, and OTHMAR MARTI — Institute of Experimental Physics, Ulm University

Concerning the constantly growing demand of advanced materials with special characteristics on nanoscale, e.g. reconfigurable nanowires, the properties and interactions of various polymers adsorbed on surfaces are still a research topic of major interest. Several methods to initiate conformational changes and reorientations are described in literature by different authors. Vapors or 2D pressure can be used to induce a collapse/decollapse cycle of single polymer chains in consequence of a coadsorption process, electric fields can be applied to align the molecules just as well as to change the surface properties of the substrate. Although the mechanisms of these observations are often analyzed, the basic driving forces are still not well understood.

In this work, novel effects of externally stimulated linear- and AB-block-copolymer chains interacting with several surfaces are presented. The molecules gain unexpectedly high mobility and show conformational changes under specific conditions and the presence of an external electric field. Varying from single molecule chains to thin polymer

films, the underlying physical effects are systematically investigated and discussed.

CPP 18.3 Tue 18:15 Poster C

IPMCs as a artificial muscle — ●PARISA BAKHTIARPOUR, MASOUD AMIRKHANI, and OTHMAR MARTI — Institute of Experimental Physics, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany

IPMCs (Ionic Polymer Metal Composite) are classified as EAPs (electro active polymers), that their properties change by electrical stimulation. The shape and size of these polymers alter when electrical voltage apply to their opposite interfaces. In additional, IPMCs bending can produce electrical signal in back movement. By patterning the metal electrodes during the IPMCs sample fabrication, movement with multiple degree of freedom is possible. The performance of IPMC can be control and monitor with several sensing methods such as surface resistivity connected in bridge configuration.

In this research, we developed Simultaneous actuating and sensing methods for IPMCs sample. We consider the sample as variable resistance which displacement of sample could be detected by proper electrical circuit design. The benefit of this method is reducing the noise and also possibility of measurement for each part of patterned sample independently.

CPP 18.4 Tue 18:15 Poster C

Annealing Effects of Thin Polymer Films and Single Chains of Poly(methyl methacrylate) on Various Substrates — ●DANIEL GEIGER, KIRSTEN DAMMERTZ, MASOUD AMIRKHANI, and OTHMAR MARTI — Institute of Experimental Physics, Ulm University

As previously stated by Guiselin [1], polymer solutions can form an irreversible adsorbed, brush-like layer on a solid interface. Napolitano and Wübbenhorst [2] concluded that the contradictory reports, concerning the dynamics of thin films, are possibly due to the formation of an irreversible adsorbed layer. Therefore, the properties of thin films are strongly dependent of the sample history, in particular of the annealing time and temperature.

The investigation of the influence of different substrates (e. g. silicon and mica) on the formation of the irreversible adsorbed layer is one of the main goals of this work, as well as the study of the temperature dependence of the irreversible adsorbed layer growth process. Furthermore, we study the behavior of single molecules on solid substrates after annealing.

[1] O. Guiselin, Irreversible Adsorption of a Concentrated Polymer Solution, *Europhys. Lett.*, 17, 225-230, 1992

[2] S. Napolitano, M. Wübbenhorst, The lifetime of the deviations from bulk behaviour in polymers confined at the nanoscale, *Nat Commun*, 2, 260, 2011

CPP 18.5 Tue 18:15 Poster C

Analysis of polymer flow in nanopores with time-resolved SAXS — ●MANUELA LUKAS and BERND STÜHN — Experimental Condensed Matter Physics, TU Darmstadt, Germany

The flow of polymers due to capillary pressure in nanopores is investigated. Polycarbonate samples are irradiated with swift heavy ions, treated with UV light and etched in NaOH solution. The nanopores are aligned strictly parallel and examined by Small-Angle X-ray Scattering (SAXS). To observe the filling behavior, time resolved SAXS measurements are performed at different temperatures.

Polydimethylsiloxane was chosen with different molecular weights. With different radii of gyration and various pore diameters a wide range of R_g/D is considered.

The filling process is shown by the steady decrease in scattering intensity with time. The whole scattering curves are fitted at every time step. It is thus possible to analyse change of intensity and form factor with time.

The intensity variation with time follows the Lucas-Washburn equation. The \sqrt{t} -dependency of the filling height is reproduced well throughout the whole filling process.

The current aim is to determine the factors that influence flow behavior in nanopores.

CPP 18.6 Tue 18:15 Poster C

Oxidation dependent magnetism in Polyvinylferrocene-b-Poly-2-Vinylpyridine diblock copolymer — ●HAIKO DIDZOLEIT¹, MARKUS GALLEI², JOHANNES ELBERT², MATTHIAS REHAHN², and BERND STÜHN¹ — ¹TU Darmstadt, Experimental Condensed Matter Physics — ²TU Darmstadt, Ernst-Berl-Institut für Technische und Makromolekulare Chemie

Switching of conformation triggered by an external stimulus is a desired ability of a variety of polymers. In focus of our research is the ferrocene containing diblock copolymer polyvinylferrocene-b-poly-2-vinylpyridine (PVFc-P2VP) with molecular weights between 8000 and 16000 g/mol⁻¹ synthesized via sequential living anionic polymerization. The first block is a hydrophilic pyridine based polymer while the second part consists of a hydrophobic polymer containing a ferrocene moiety. This moiety has a strong influence on the properties such as magnetism, dynamic and solubility. SQUID measurements reveal that the magnetic susceptibility of the polymer can be changed by an oxidation agent from diamagnetic to paramagnetic. This effect depends on the characteristics of the polymer such as oxidation ratio and chain length. Furthermore the oxidation effects the conformational structure of the diblock copolymer which we investigate using X-Ray diffraction. The amphiphilic property enables the polymer to be analyzed as a monolayer on solid substrates as well as dissolved on a liquid surface, this gives the opportunity to change polymer conformation dependent on the mean molecular area. Results from the X-Ray reflectometry reveal a dependency of the layer thickness regarding oxidation.

CPP 18.7 Tue 18:15 Poster C

Entropic DNA segregation in bacteria — ●ELENA MININA and AXEL ARNOLD — Institute for Computational Physics, University of Stuttgart, Allmandring 3, 70569, Stuttgart, Germany

Cell division is a complex process consisting of two main parts - DNA replication and segregation. In all higher organisms, both parts involve active mechanisms. In particular, the mechanism for segregation is too complex to be employed by primitive bacteria like *Escherichia coli*. During replication DNA of the mother cell is copied into two daughter strands, which segregate, i.e. move towards opposite sides of the rod-shaped cell. It was previously shown that the segregation can be driven by entropy only, without need for an active mechanism [A. Arnold and S. Jun, Phys. Rev. E 76 (2007)]. The time scale for this entropic segregation is much faster than simple diffusion, and sufficient to explain DNA segregation in primitive bacteria. However, there is barrier towards entropic segregation, which has to be overcome by diffusion and would be a major obstacle towards purely entropic segregation.

In the present study we use MD simulations in order to investigate the influence of finite replication speed on the segregation. We model the replication by unzipping of two initially cross-linked, ladder-like strands, and compare to a more realistic model, where a second strand is added gradually. Our results show that the finite replication speed allows to overcome the induction time, which is only an artifact of spontaneous segregation. Without the need for induction, entropic segregation is indeed a promising candidate to explain bacterial DNA

segregation without active mechanisms.

CPP 18.8 Tue 18:15 Poster C

Passive and active microrheology of a polymer melt studied by molecular dynamics simulation — ●ANJA KUHNHOLD and WOLFGANG PAUL — Institut fuer Physik, Martin-Luther-Universitaet, 06099 Halle

The rheology of polymer melts can be observed from the behaviour of suspended particles (microrheology). Therefore MD simulations of a bead-spring polymer melt model including one or two nanoscopic particles are carried out. Passive microrheology yields linear response properties of the polymer melt by looking at the thermal motion of the nanoparticles. From the mean square displacement of the nanoparticles the complex modulus $G^*(\omega)$ of the melt is determined by using a generalized Stokes-Einstein equation. Results for one- and two-particle microrheology are compared. Furthermore the nonlinear response of the polymer melt is investigated by applying forces to the melt. Here a nanoparticle-oscillator is used; i.e. two nanoparticles are connected by a harmonic potential and the compressed oscillator is put into the polymer melt. The resulting oscillation of the nanoparticles is studied for different melt temperatures and different spring constants.

CPP 18.9 Tue 18:15 Poster C

Growth process of monodisperse cylindrical polymer micelles measured by SAXS, DLS and TEM — ●CHRISTINA LEDERLE¹, JOHANNES ELBERT², MARKUS GALLEI², MATTHIAS REHAHN², and BERND STÜHN¹ — ¹Experimental Condensed Matters Physics, TU Darmstadt, Germany — ²Makromolekulare Chemie, TU Darmstadt, Germany

Cylindrical micelles are grown on the basis of seeds formed by aggregates of the block copolymer polyferrocenylsilane-b-poly(dimethylsiloxane) (PFS-b-PDMS) in hexane (selective for the second block). The seeds were produced by 4 hours sonication. Adding a second block copolymer (Polyisoprene-b-PFS) in Tetrahydrofuran (good solvent for both blocks) to these seeds cylindrical micelles are grown. Their length depends on the addition of a specified amount of PI-b-PFS in THF.

We study these aggregates with Dynamic Light Scattering (DLS) and Transmission Electron Microscopy (TEM). TEM - pictures show a big length difference between PFS-b-PDMS seeds after applied 4 hours sonication (40 - 60 nm) and grown cylinders (200 nm - 1000 nm). Diffusion coefficients, measured by DLS, decrease with increasing addition of further chains. Furthermore we observe the growth process via measured intensity in light scattering experiments, started from seeds and added PI-b-PFS in solution during the measurement. The intensity increases until a plateau appears after days.

We plan to orientate those grown cylinders in solution via application of an electric field and measure its effect by SAXS.

CPP 18.10 Tue 18:15 Poster C

Neutron Scattering and Simulations on Polymers confined in Silica Nanopores — ●MATTHIAS MUTHMANN, REINER ZORN, and DIETER RICHTER — Jülich Centre for Neutron Science JCNS and Institute for Complex Systems ICS Forschungszentrum Jülich GmbH, Germany

We will present neutron scattering experiments on confined polymers. The confinement was realized by nanoporous silica. It consists of silica particles (\varnothing approx. 2 μ m) that are covered by hexagonal pores with a diameter of approximately 5nm. These pores channel through the whole particle and can be filled with the polymer. A neutron backscattering measurement has been performed at the SPHERES instrument and a complementary time of flight experiment at the TOFTOF instrument. Both are located at the FRM2 reactor in Munich. We discovered a significant slowdown of the local dynamics of the confined polymer. To investigate the chain dynamics, we did a the measurement at the neutron spin echo spectrometer at Oak Ridge National Laboratory. The experiment yielded a slowdown of the dynamics of the whole chain.

The spectra obtained from our neutron scattering experiments have been compared to the results from atomistic simulations. We created a system of polymer chains, confined in a silica nanopore, similar to the system of our experiments. For this purpose, we used the commercial software Discover by Accelrys. The simulations yielded trajectory files of the simulated polymer chains. These trajectories then allowed a comparison to experimental results.

CPP 18.11 Tue 18:15 Poster C

A Detailed Study on Heterogeneous Dynamics in Polymers Close to Tg by SM Techniques — ●SUBHASIS ADHIKARI, MARKUS SELMKE, and FRANK CICHOS — Inst. of Expt. Physics I, University of Leipzig, Germany

The temperature dependent rotational dynamics of a single perylene dimide (PDI) dye molecule in Poly (methyl acrylate) (PMA) and in poly (vinyl acetate) (PVAc) have been studied. The autocorrelation of linear dichroism (LD) of a single PDI molecule is stretched exponential. The dynamics of a single probe molecule is temporally heterogeneous. The rotational times and stretching exponents are widely distributed. All SM results are discussed using a simple model of dynamical heterogeneity based on a Gaussian distribution of activation energies. SM average rotational times follow Debye - Stokes - Einstein (DSE) law for polymer viscosity. Dielectric measurements shows that probe rotation may or may not couple to segmental motion. Probe with different size follow same temperature dependence as predicted from DSE law.

Detailed information on heterogeneous dynamics is further expected from an extension of two - point nanorheology to single molecule optical studies based on fluorescence resonance energy transfer (FRET). We have therefore synthesized bi - labeled (Alexa 488 and Alexa 594) polystyrene polymer. Lifetime and intensity based smFRET are reported.

CPP 18.12 Tue 18:15 Poster C

Study of PEG loaded Nonionic Microemulsions using DLS — ●PHILIPP GRAMLICH, ANDREAS BISCHOF, ANDREAS WEBER, and BERND STÜHN — Experimental Condensed Matter Physics, TU Darmstadt

We study the behaviour of polymer loaded nonionic w/o-microemulsions in droplet phase using dynamic light scattering methods. The microemulsions are water-C12E4-octane mixtures with different concentrations of PEG 1500. We keep a steady relation $\omega = 10$ between water molecules per surfactant molecules as well as a constant volume fraction $\phi = 0.1$ of water plus surfactant to total volume while varying the polymer content. Experiments are performed in a temperature range from 10 to 70 degrees Celsius. Coefficients of translational and rotational diffusion are measured and used to compute hydrodynamic radii. Special attention is given to the possible change between droplets and lamellar/bicontinuous structures in the proximity of phase transitions. Additionally we performed SANS and SAXS as well as transmissional and dielectric measurements.

The addition of PEG 1500 strongly affects the hydrodynamic radii extracted by DLS. Furthermore the hydrodynamic radii differ greatly for different temperatures which cannot be explained solely by a change of viscosity for any of the components.

CPP 18.13 Tue 18:15 Poster C

Novel thermoresponsive polymers in various architectures — ●KONSTANTINOS KYRIAKOS¹, SARAH OTTINGER¹, ANNA MIASNIKOVA², ANDRÉ LASCHEWSKY², PETER MÜLLER-BUSCHBAUM¹, and CHRISTINE M. PAPADAKIS¹ — ¹TU München, Physikdepartment, Physik weicher Materie, Garching — ²Universität Potsdam, Fakultät für Chemie, Potsdam-Golm

Amphiphilic copolymers with a thermoresponsive block have attracted interest, mainly because of their ability to self-assemble into micelles with a thermoresponsive shell in water. Poly(methoxy diethyleneglycol acrylate) (PMDEGA) is a new thermoresponsive polymer, which exhibits critical temperatures in the range 35-45 °C.

We report here on fluorescence correlation spectroscopy (FCS) experiments on various PMDEGA-PS systems, focusing on the effect of the different molecular architectures. We studied a P(S-*b*-MDEGA) diblock, a P(S-*b*-MDEGA-*b*-S) triblock and a (P(MDEGA-*b*-S))₃ three-arm star copolymer. Information about the critical micelle concentration (CMC) and the hydrodynamic radius (r_H) were obtained. In agreement with our previous results [1], we observe a strong dependence of the different chain architectures on the CMC of the studied systems. Moreover, the r_H of the micelles varied with chain architectures.

[1] A. Miasnikova, A. Laschewsky, C.M. Papadakis, P. Müller-Buschbaum, et al., *Langmuir* (2012), 28, 4479

CPP 18.14 Tue 18:15 Poster C

Cononsolvency of PNIPAM in water/methanol mixed solutions — ●KONSTANTINOS KYRIAKOS¹, MARTINE PHILIPP¹, JOSEPH ADELBERGER¹, SEBASTIAN JAKSCH¹, ANNA MIASNIKOVA², ANDRÉ LASCHEWSKY², ISABELLE GRILLO³, PETER MÜLLER-BUSCHBAUM¹, and CHRISTINE M. PAPADAKIS¹ — ¹TU München, Physikdepartment,

Physik weicher Materie, Garching — ²Universität Potsdam, Fakultät für Chemie, Potsdam-Golm — ³Institut Laue-Langevin, Grenoble, France

Thermoresponsive polymer poly(N-isopropyl acrylamide) (PNIPAM) exhibits a lower critical solution temperature (LCST) of 32 °C in aqueous solution. Upon the addition of a second polar solvent, e.g. methanol, a miscibility gap appears, which is termed as cononsolvency. Diblock copolymers consisting of a long PNIPAM block and a short polystyrene block, e.g. P(S-*b*-NIPAM), form micelles with a thermoresponsive shell [1].

We report here on a stopped-flow experiment with time-resolved SANS on an aqueous solution of a PNIPAM homopolymer or a P(S-*b*-NIPAM) diblock copolymer to which methanol was added. This resulted in a collapse transition of the linear chains or the micellar shell, respectively, and on the subsequent aggregation. For both systems the aggregation path and the final size of the formed aggregates depend on the mixing ratio. Interestingly, the size of the formed aggregates is much bigger for the homopolymer compared to the diblock copolymer.

[1] J. Adelsberger, A. Laschewsky, P. Müller-Buschbaum, C.M. Papadakis et al., *Colloid Polym. Sci.* 2011, 289, 711

CPP 18.15 Tue 18:15 Poster C

Synthesis and dynamic studies of H-bonded double networks — ●BARBARA GOLD, WIM PYCKHOUT-HINTZEN, CLAAS HÖVELMANN, JÜRGEN ALLGAIER, ANA BRAS, ANDREAS WISCHNEWSKI, and DIETER RICHTER — Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS-1) & Institute of Complex Systems (ICS-1), 52425 Jülich

In the framework of a recently granted EU project on SelfHealing Innovative Elastomers (SHINE) newly developed elastomers containing both permanent and/or transient crosslinks in different concentrations in rubbers will be investigated by different measurement methods.

The chemical concept of SHINE involves two types of linkages in the molecular structure of the self-healing elastomers: strong covalent bonds that do not undergo reversible changes to provide strength and rigidity to the material and transient bonds that thermodynamically can be broken. Re-combination of the broken segments will result in the novel self-healing properties.

We present the synthesis of our model network, which consists of monodisperse polydienes (PI) where the backbone and extremities are modified with H-bonding active groups. Furthermore first results of rheological experiments will be shown to get a basic impression of how chain dynamics change due to the networking process and will be influenced of thus permanent and transient crosslinks with respect to self-healing mechanism.

CPP 18.16 Tue 18:15 Poster C

POCLMD: A Flexible GPU Accelerated Molecular Dynamics Code — ●CHUANFU LUO¹ and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden, Germany — ²Technische Universität Dresden, Germany

Recently, general-purpose computing on Graphics Processing Units (GPU) or coprocessor cards becomes a trend in high performance computing. Many newly built super-computers are equipped with powerful GPUs or coprocessors. Currently, several companies provide high performance accelerating cards and all of them support the open standard OpenCL programming. The code writing in OpenCL can run on multiple-core CPUs, GPUs, and coprocessors without any changes. POCLMD is designed to be a fast, flexible and easy-to-use MD code, which is programmed in Python and OpenCL through Py-OpenCL [1]. The kernel code written in OpenCL is compiled and loaded on the fly during the running, thus the executing kernel of POCLMD is very small and efficient. Benefited by the powerful template programming of Python, POCLMD can support an easy and flexible way to add some custom potentials without asking users to modify the codes. The first benchmark of LJ liquids shows that the performance of POCLMD can catch up 90% of HOOMD-blue [2] (the fastest CUDA based MD code) on the same NVIDIA's GPUs. The best performance is achieved on an AMD's HD7970 card, on which POCLMD runs over 80 times faster than LAMMPS on a single core Q6600 CPU (2.4GHz). [1] <http://mathematician.de/software/pyopencl> [2] <http://codeblue.umich.edu/hoomd-blue/>

CPP 18.17 Tue 18:15 Poster C

Molecular Dynamics and Conductivity of Solid Polymer Electrolytes based on Poly(butylene)oxide and LiClO₄ — ●BERNHARD HOPFENMÜLLER¹, GERALD SCHNEIDER¹, JÜRGEN

ALLGAIER², REINER ZORN², and DIETER RICHTER² — ¹Jülich Center for Neutron Science JCNS, Forschungszentrum Jülich GmbH, Outstation at FRM II, Lichtenbergstr.1, 85747 Garching — ²Institute of Complex Systems (ICS-1) and Jülich Center for Neutron Science (JCNS), Forschungszentrum Jülich GmbH, 52425 Jülich

Solid polymer electrolytes play a crucial role in our daily life, e.g. as polymer-based batteries. Such systems are build up of mixtures containing a polymer and a salt. The charge carrier mobility and therefore the conductivity is inherently coupled with the molecular dynamics of the polymer itself. Addition of salt changes the stiffness of a polymer and hence again the conductivity is affected. The most simple and therefore much studied systems are based on poly(ethylene)oxide. This polymer crystallizes at ambient temperature. Though solid polymer electrolytes based on it have a reduced conductivity in solid state. Therefore we wanted to study systems based on poly(butylene)oxide (PBO) and lithium perchlorate (LiClO₄). PBO has an additional side-group that prevents crystallization at all temperatures. Dielectric spectroscopy allows to study both, conductivity and molecular dynamics with the same technique. In our presentation we want to show results of dielectric spectroscopy on solid PBO electrolytes with different salt contents. We want to demonstrate that the conductivity and the molecular dynamics are mainly coupled by the segmental dynamics.

CPP 18.18 Tue 18:15 Poster C

Dielectric spectroscopy on polymer loaded microemulsions based on C12E4 — ●ANDREAS BISCHOF, ANDREAS WEBER, CHRISTINA LEDERLE, and BERND STÜHN — Experimental Condensed Matter Physics, TU Darmstadt

We study the droplet phase of pure and polymer loaded nonionic w/o microemulsions composed of the surfactant C12E4 by the combination of different experimental methods, e.g. light transmission, dielectric spectroscopy and SAXS.

For different droplet sizes and concentrations the phase behaviour and structure are well understood. It is known that the addition of a polymer to a microemulsion may change structure and dynamic of the droplets. For an investigation of the effect on dynamics we compare the dielectric spectra of the pure microemulsion and of microemulsions loaded with the water soluble PEG. We found several relaxations, varying in relaxation time and strength, depending on the structural and dynamical changes and applied temperature.

Further we observe a strong effect of system composition and polymer concentration on the stability of the droplet phase. We will discuss the dielectric relaxations in pure and polymer loaded systems.

CPP 18.19 Tue 18:15 Poster C

The Jülich Neutron Spin Echo Spectrometer: Dynamics with Depth Resolution — ●OXANA IVANOVA¹, OLAF HOLDERER¹, and MICHAEL MONKENBUSCH² — ¹Jülich Centre for Neutron Science, Forschungszentrum Jülich, Aussenstelle am FRM II, Garching — ²Jülich Centre for Neutron Science, Forschungszentrum Jülich, Jülich, Germany

Neutron spin-echo (NSE) spectroscopy is a neutron scattering technique with the highest energy resolution. It enables investigation of very slow dynamic processes and via scattering vector gives access to the spatial information. The accessible time and length scales are relevant for observation of thermal fluctuations in mesoscopic systems. High energy resolution, low background and good instrumental stability of J-NSE spectrometer at FRM II research reactor in Garching enables the use of grazing incidence technique (GINSES). Along with conventional NSE spectroscopy, GINSES is developed to be used as 'push-button' option to resolve depth dependent near surface dynamics. Scientific applications of J-NSE instrument include dynamics of classical and critical microemulsions, microgels, polymer blends, polymers in solution and different confinement, membranes and so on. Some examples of recent experiments will be presented.

CPP 18.20 Tue 18:15 Poster C

Huge material transport in azobenzene polymer films induced by highly intense laser light of 534 nm — ●ZAHRA MOLLA¹, REGINA ROSENHAUER², JOACHIM STUMPE², and ULLRICH PIETSCH¹ — ¹Universität Siegen, Festkörperphysik, Siegen, Germany — ²FHI für Angewandte Polymerforschung, Potsdam, Germany

Photochemical polymers undergo permanent trans to cis isomerisation under illumination with UV or visible light. In the past this property has been used to generate surface relief lattices via illumination of thin films of an azobenzene polymer, for example, by an interference

pattern of polarized light. For this purpose typically Ar⁺ lasers emitting at 488nm with power < 250mW have been used. Meanwhile new lasers, such as disc lasers emitting at 534nm, are available with beam power up to 2W. In order to study light induced nano-movement, a thin film of the photopolymer Holomix5 was irradiated under normal incidence by an expanded beam of the disc laser. The induced change in film height has been probed by He-Ne laser (633nm) under an angle of 30°. Recorded by a photo diode the reflected intensity shows dramatic changes while illumination. The intensity increases immediately by several percent switching the disc laser with power > 500mW on followed by intensity oscillation with time period of few seconds. The intensity drops back to the initial values switching the disc laser off. The number of oscillations depends on laser power. The scattering data are interpreted in terms of Fresnel equations and refer to the creation of a column formed by polymer material with height up to several 100nm and column diameter equal to that of the laser beam.

CPP 18.21 Tue 18:15 Poster C

Li-dynamics in amorphous PEO electrolytes in supercooled liquid states — ●JOYJIT CHATTORAJ, DIDDO DIDDENS, and ANDREAS HEUER — Institute of Physical Chemistry, Westfälische Wilhelms-Universität Münster, Corrensstr. 28/30, D-48149 Münster, Germany

The effect of ionic liquids on Li-dynamics is investigated via MD simulation in a poly(ethylene oxide) PEO-based polymer electrolyte material containing Li-TFSI salt and MPPY-TFSI ionic liquid (IL) for a vast temperature regime ranging from above the freezing temperature to the vicinity of the glass transition temperature of PEO. Li cations are complexed with ether oxygen atoms and move via continuous bond breaking and making. Three key mechanisms of cation transport in polymer melts had already been identified at temperatures well above the freezing point. These are M1: intrachain motion, M2: segmental motion and M3: interchain motion. In addition, a plasticizing effect of ionic liquid had been noticed by Diddens et al [arXiv:1211.3413]. In this paper we show that the three mechanisms also hold for low temperatures and a simple Rouse model could be applied to explain these mechanisms as done in the case of high temperature polymer melt. The plasticizing effect of ionic liquid diminishes as we find that the diffusion coefficient of Li tends to collapse for all IL concentrations while approaching the glass transition.

CPP 18.22 Tue 18:15 Poster C

Rheology of Complex Fluids: Mathematical Modeling — ●JOSE MANUEL MUNOZ VILLEGAS — Universidad de Guadalajara, Guadalajara, Mexico

In this work is introduced the SMV model. This model mixes Giesekus model and Johnson-Segalman model. Dynamic simulations (shear stress) are showed under steps shear rate. First and second normal stress differences are also showed. This model predicts well steady and unsteady nonlinear flow.

CPP 18.23 Tue 18:15 Poster C

Dynamic consequences of missing chain ends — ●SEBASTIAN GOOSSEN, ANA RITA BRÁS, WIM PYCKHOUT-HINTZEN, ANDREAS WISCHNEWSKI, MARGARITA KRUTYEVA, JÜRGEN ALLGAIER, and DIETER RICHTER — Jülich Centre for Neutron Science, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

The dynamics of cyclic polyethylene glycol (PEG) in a melt was studied by neutron spin echo spectroscopy (NSE) and PFG-NMR for three distinct molecular weights. In comparison with their linear analogs the ring polymers showed a significantly faster center of mass diffusion. This turns out to be an explicit violation of the Rouse model for the smallest rings (~1 Me). Slightly bigger rings (~3 Me) fulfill the Rouse behavior perfectly taking into account the different mode structure due to the ring architecture, while linear chains are already slowed down due to the onset of entanglements. For even bigger rings (~5 Me) the Rouse dynamics does not apply anymore. Obviously topological ring-ring-interactions lead to slower dynamics. However, while for linear chains these topological interactions can be described by entanglements, for the rings they are still not fully understood. Further studies dealt with blends of cyclic and linear PEG. Cyclic polymers in a linear matrix are slowed down effectively with increasing chain length of the linear matrix. On the other hand slightly entangled linear chains (~3 Me) in a matrix of cyclic polymers of the same molecular weight diffuse much faster than in a linear environment. This very first molecular weight dependent case study on the dynamics of ring polymers in the melt is compared to recent simulation work.

CPP 18.24 Tue 18:15 Poster C

Switching single macromolecules at modified graphene surfaces — •CHIEN-LI LEE¹, DAVID BLÉGER², STEFAN HECHT², and JÜRGEN RABE¹ — ¹Institut für Physik, Humboldt-Universität zu Berlin — ²Institut für Chemie, Humboldt-Universität zu Berlin

Introducing azobenzene moieties into polymers has recently been shown to allow for optically switching the aggregation behavior of the polymer in solution, which has been attributed to rod-coil transitions [1]. Due to the difficulty of isolating single switchable azobenzene-containing polymers on solid substrates, they were studied so far in aqueous solutions, thin films and bulk materials, thereby reflecting ensemble properties.

Here we present an approach to switch single macromolecules immo-

bilized on a modified graphene surface. A synthetic rigid-rod polymer [1] incorporating azobenzene photoswitches in the backbone was deposited from aqueous solution onto a graphite surface precoated with an oriented monolayer of octadecylamine [2]. Single rod-like polymers aligned by the substrate have been imaged by scanning force microscopy. Photoisomerization back and forth between trans and cis at different wavelengths leads to shrinking and stretching, respectively, as well as some local movements of the macromolecules on the surface.

[1] David Bléger, T. Liebig, R. Thiermann, M. Maskos, J. P. Rabe, and S. Hecht *Angew. Chem. Int. Ed.* 2011, 50, 12559.; [2] N. Severin, I.M. Okhupkin, A.R. Khokhlov, and J.P. Rabe, *Nano Lett.* 2006, 6 1018

CPP 19: Poster: Crystallization, Nucleation and Self Assembly

Time: Tuesday 18:15–20:15

Location: Poster C

CPP 19.1 Tue 18:15 Poster C

The formation of polymeric honeycomb structure in the presence of different organic liquids — FARID FARAJOLLAHI, MASOUD AMIRKHANI, and •OTHMAR MARTI — Institute of Experimental Physics, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany

Micro porous polymer structures have several applications in photonic devices, cell culturing scaffolds and super hydrophobic surfaces. Recently, self assembly of polymers into micro structures have gained more attention and different methods have been suggested for fabrication desirable patterns. Condensation of water on a volatile polymeric solution which called Breath Figure is one of the new method to produce order micro structure. The ability to make order bubble pattern with one step process have provided unique properties for breath figure method.

In this research, we made the micro bubble structure by adding a small amount of different organic liquid to linear polystyrene solution. By adjusting the concentration of organic liquid, the shape and structure of honeycomb pores can be tuned. For different organic liquid, the effect of length of carbon chain on the self assembled pattern have been investigated

CPP 19.2 Tue 18:15 Poster C

Transcrystallinity in isotactic polypropylene: synchrotron IR microspectroscopy and microfocus X-ray scattering — •GONZALO SANTORO¹, SHUN YU¹, STEPHAN V. ROTH¹, ULRICH SCHADE², and GARY ELLIS³ — ¹HASYLAB at DESY, Notkestr. 85, 22607, Hamburg, Germany. — ²BESSY-II, Helmholtz-Zentrum Berlin, Albert-Einstein-Str. 15, 12489, Berlin, Germany. — ³Institute of Polymer Science and Technology, ICTP-CSIC, Juan de la Cierva 3, 28006 Madrid, Spain.

Isotactic polypropylene (iPP) is one of the most widely-used consumer polymers. It is a semicrystalline thermoplastic exhibiting four different polymorphs: the monoclinic α phase (thermodynamically the most stable and predominant under regular processing conditions), the trigonal β phase (promoted under special processing conditions, like crystallization under shear), the orthorhombic γ phase (present in materials with low molecular weight or regular chain defects) and a mesomorphic phase (a semi-ordered phase) [1]. Moreover, when crystallization takes place in the presence of fibers, transcrystalline morphologies can develop.

This work presents polarization modulated synchrotron IR microspectroscopy and microfocus X-ray scattering studies on the transcrystalline β -cylindric phase of iPP, showing evidence for lamellar twisting along the growth direction [2,3].

[1] B. Lotz et al. *Polymer* **37**, 22, 4979 (1996).

[2] J. Torre et al. *Macromolecules* **39**, 16, 5564 (2006).

[3] G. Santoro et al. *J. Phys.: Conf. Ser.* **359**, 012005 (2012).

CPP 19.3 Tue 18:15 Poster C

Unusual crystallization kinetics in poly(1,1-dimethyl silacyclobutane) — •JUNYU LI¹, SCHÖNBERGER ASTRID², KUTTICH BJÖRN¹, JOHANNES ELBERT², GALLEI MARKUS², STÜHN BERND¹, and REHAHN MATTHIAS² — ¹Experimental Condensed Matter Physics, TU Darmstadt — ²Ernst-Berl-Institute for Technical and Macromolecular Chemistry, TU Darmstadt

The crystallization behavior of poly(1,1-dimethyl silacyclobutane)

(PDMSB) with molecular weight ranging between 3.000 and 50.000 kilodalton has been studied through Small Angle X-ray Scattering (SAXS), X-ray Diffraction (XRD) and Differential Scanning Calorimetry (DSC). Well-defined PDMSB homopolymers with polydispersity index less than 1.2 have been prepared by living ring-opening anionic polymerization. It has been found that in the cooling process only one crystallization peak was observed by DSC, however, in subsequent heating process two obvious melting peaks appeared. SAXS results show that there is only one long range order. DSC measurements also show that when isothermal crystallization temperature T_c is low enough, there will be two melting peaks, but only one melting peak when T_c is high. The value of lower melting peak T_{m1} increases with T_c , showing the increase of lamella thickness due to increase of T_c . However, the value of higher melting peak T_{m2} stays constant with T_c . In addition, surface-attached PDMSB on polystyrene particle was studied. DSC results show that only one melting peak was observed independent of T_c . Based on these observations, re-crystallization is suggested to explain this interesting phenomenon.

CPP 19.4 Tue 18:15 Poster C

Effect of Shear Stress on Crystallization of Isotactic Polypropylene from a Structured Melt — •BIN ZHANG^{1,2,3}, JINGBO CHEN³, BARBARA HECK¹, and GÜNTER REITER¹ — ¹Institute of Physics, University of Freiburg, Germany — ²Hermann Staudinger Graduate School, University of Freiburg, Germany — ³School of Materials Science & Engineering, Zhengzhou University, Peoples Republic of China

Based on a control of the melt structure at temperatures near but below the equilibrium melting point we investigated the role of shear stress imposed by the wall of the capillary die on crystal morphology of isotactic polypropylene (iPP). The nanoscale bundles of partially ordered chain segments within the quiescent melt at temperatures between the nominal melting temperature (T_m) and the equilibrium melting point (T_m^0) allowed for the possibility of shear-induced or shear-assisted formation of crystalline cylindrites which were investigated by means of polarized optical microscopy and small/wide-angle X-ray scattering. The SAXS patterns of near melting point structured melt monitored at 180 °C can be fitted by using a form factor for polydisperse cylinders. It was found that the average radius and height of the bundles of partially ordered chain segments was about 17 nm and 40 nm, respectively. For a given structured melt, the number of cylindrites increased with shear stress, concomitantly, the nucleation density of α -iPP within a single cylindrite structure increased with shear stress at the expense of β -iPP nucleation density.

CPP 19.5 Tue 18:15 Poster C

MUSIC-mode AFM of self-assembled oligothiophene fibrils — •MARTIN FEIFER¹, EIKE-CHRISTIAN SPITZNER¹, ROBERT MAGERLE¹, ROMAN MARTY², and HOLGER FRAUENRATH² — ¹Chemische Physik, TU Chemnitz, D-09107 Chemnitz — ²Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland

We investigate the structure of self-assembled oligothiophene fibrils, that may be of interest as organic semiconducting nanowires. Spin-coated on a substrate, the fibrils are about 26 nm wide and have an average height of 2.9 nm. For analysis we use multi-setpoint intermittent contact (MUSIC) mode atomic force microscopy (AFM), which provides with unprecedented spatial resolution data on the fib-

rials nanomechanical properties and gives a detailed insight into the inner structure. The fibrils consist of a rigid core from tetrathiophene terminally attached with oligopeptides that form a soft shell. We also present results on different substrates and discuss their influence on the fibril's configuration. Furthermore we compare results using standard AFM tips to high-resolution data, obtained by super sharp AFM tips.

CPP 19.6 Tue 18:15 Poster C

Free energies of fcc, hcp, and bcc phases of hard sphere crystals — ●MOHAMMAD HOSSEIN YAMANI and MARTIN OETTEL — Institut für Angewandte Physik, Universität Tübingen, Germany

We use density functional theory of fundamental measure type (FMT) to evaluate the fully unconstrained minimized periodic fcc, hcp and bcc crystal profiles. Previous FMT results in the case of fcc compare very well to simulation results [1]. hcp and fcc differ only in the stacking sequence of hexagonally packed planes of particles, and thus one expects only a small free-energy difference between these two structures. FMT predicts hcp to be more stable than fcc by a free energy difference per particle of the order of $0.001 k_B T$. Instead, simulation results show that fcc is more stable than hcp by about the same free energy difference. We rationalize these findings using Stillinger's expansion [2] for the crystal partition function in the number n of correlated, free particles in a matrix of frozen particles at ideal lattice positions. It turns out that the stability of hcp over fcc holds for a truncation at $n = 2$, giving approximately the same hcp-fcc free energy difference as FMT. For a reversal of stability truncation at higher n is required.

[1] M. Oettel et al., Phys. Rev. E 82, 051404 (2010).

[2] W. G. Rudd et al., J. Chem. Phys. 49, 4857 (1968).

CPP 19.7 Tue 18:15 Poster C

Crystalline microstructure of thin elastomeric polypropylene films — ●JULIA SEEMANN, MARTIN NEUMANN, and ROBERT MAGERLE — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

Elastomeric polypropylene (ePP) is a semi-crystalline polymer with a low degree of crystallinity of $< 20\%$. We study with atomic force microscopy (AFM) the crystalline microstructures forming in thin films of ePP crystallised from solution or melt. One objective is to find ideal conditions for the formation of the crosshatch structure. The films were prepared on silicon substrates via spin coating or dip coating and were annealed under inert conditions for a few hours up to 4 weeks at temperatures between 90°C and 150°C . With dip coating, gradient films have been prepared, showing a continuous increase in film thickness over the lateral extent. This allows for correlation of the film thickness with the crystalline microstructure. With increasing film thickness the size of hedrites decreases and their number increases. The degree of crystallinity depends on the annealing temperature and time, which is in line with general trends reported in the literature.

CPP 19.8 Tue 18:15 Poster C

Polymer blend lithography: A versatile method for fabricating nanopatterned self-assembled monolayers — CHENG HUANG^{1,2}, MARKUS MOOSMANN^{1,2}, JIEHONG JIN^{1,2}, TOBIAS HEILER^{1,2}, ●PAUL VINCZE^{1,2}, STEFAN WALHEIM^{1,2}, and THOMAS SCHIMMEL^{1,2} — ¹Institute of Nanotechnology, Karlsruhe Institute of Technology — ²Institute of Applied Physics and Center for Functional Nanostructures, Karlsruhe Institute of Technology

Polymer blend lithography is introduced as a rapid method to produce patterned self-assembled monolayers on solid substrates featuring different chemical functionalities. For the pattern generation the phase separation of two immiscible polymers, polystyrene (PS) and poly(methylmethacrylate) (PMMA), as a blend solution is used for coating by a spin-coating process. By controlling the spin-coating parameters and conditions, including the humidity, the molar mass of the PS and PMMA, and the mass ratio between the two polymers in the blend solution, the formation of a purely lateral morphology can be reproducibly induced. By selectively dissolving one component, a monolayer copy of the corresponding polymer phase morphology can be created. The patterning process is applied with various functional molecules forming self-assembled monolayers (SAM). This process is

suitable for the rapid preparation of quasi two-dimensional nanopatterned functional substrates [1].

[1] Huang, C.; Moosmann, M.; Jin, J.; Heiler, T.; Walheim, S.; Schimmel, T. Beilstein J. Nanotechnol. 2012, 3, 620-628. doi:10.3762/bjnano.3.71

CPP 19.9 Tue 18:15 Poster C

Deformation mechanisms in semi-crystalline polymers investigated by x-ray scattering — ●KONRAD SCHNEIDER — Leibniz-Institut für Polymerforschung Dresden, Germany

Depending on the molecular structure the crystallization behaviour of different polymers is different. This is the reason for differences also in the deformation mechanisms of these materials. The lecture compares the deformation mechanisms of different polymers investigated by simultaneous synchrotron small and wide angle scattering during deformation.

CPP 19.10 Tue 18:15 Poster C

Control over crystallization and crystallite orientation in conducting polymer blend films — ●EVA M. HERZIG¹, AMMARA AKTHAR¹, ANNA NAUMANN¹, CLAUDIA M. PALUMBINY¹, WEIJIA WANG¹, SHUAI GUO¹, GREGORY TAINTER¹, JAN PERLICH², SHUN YU², STEPHAN V. ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany — ²HASYLAB at DESY, 22603 Hamburg, Germany

Various parameters can be exploited to influence the morphology and therefore the performance of conducting polymer blends used in photovoltaic applications [1]. In particular charge transport is anisotropic in many conducting polymers and hence is sensitive to molecular orientation and presence of crystalline domains. Therefore it is highly desirable to have control over crystallization and crystallite orientation. We demonstrate for the well-studied system P3HT:PCBM the response of molecular ordering to the addition of two different passive components. The thorough investigation of these systems, using advanced scattering techniques, spectroscopy and microscopy measurements, allow us to select well-defined preparation protocols to deliberately choose the predominant orientation of crystalline domains in the thin conducting polymer blend films.

[1] M. A. Ruderer, and P. Müller-Buschbaum, Soft Matter 7, 5482 (2011)

CPP 19.11 Tue 18:15 Poster C

Structure and Dynamics of self-healing model polymers in the melt — ●ANA RITA BRÁS, MARGARITA KRUTYEVA, WIEBKE ANTONIUS, CLAAS HÖVELMANN, JÜRGEN ALLGAIER, WIM PYCKHOUT-HINTZEN, ANDREAS WISCHNEWSKI, and DIETER RICHTER — Forschungszentrum Jülich, JCNS-1/ICS-1, D52425 Jülich, Germany

One fascinating aspect of a self-assembly of supramolecular polymers carrying functional endgroups is the possibility of controlling the structure, adding functionalities, adjusting the macroscopic properties and taking profit of the non-trivial dynamics associated to the reversibility of hydrogen bonds. The most recent application of these polymers is the self-healing ability. Models of such materials have been synthesized, in which appropriate end-functionalization was performed by using DNA-inspired end-groups like Thymine(Thy)(A) and Diaminotriazine (Triaz)(B). These homoditopic mixtures AA/BB build exclusively key-lock systems A-B. The pre-polymer was polyethylene(glycol)(PEG). Both, Small Angle Neutron Scattering and Neutron Spin-Echo Spectroscopy were performed in the melt allowing to quantitatively access the assembly process. The structure was described for the first time by a Random Phase Approximation generalized to multiblock copolymers consisting of H and D based hydrogen-bonded supramolecular copolymers including interactions. Moreover, it was shown that by NSE the dynamics of hydrogen bonded macromolecules can indeed be accessed. The results could be described in terms of a significantly changed mode structure of the supra-chain based on the suppression of long wavelength Rouse modes. Supported by DFG-SPP1568 and EU-Dynacop

CPP 20: Poster: Colloids and Complex Liquids

Time: Tuesday 18:15–20:15

Location: Poster C

CPP 20.1 Tue 18:15 Poster C

Many-body effects for critical Casimir forces — ●THIAGO MATTOS^{1,2}, LUDGER HARNAU^{1,2}, and SIGFRIED DIETRICH^{1,2} — ¹Max Planck Institute for Intelligent Systems, Stuttgart, Germany — ²IV. Institute for Theoretical Physics, Stuttgart University, Stuttgart, Germany

Within mean-field theory we calculate the scaling functions associated with critical Casimir forces for a system consisting of two spherical colloids immersed in a binary liquid mixture near its consolute point and facing a planar, homogeneous substrate. For several geometrical arrangements and boundary conditions we analyze the normal and the lateral critical Casimir forces acting on one of the two colloids. We find interesting features such as a change of sign of these forces upon varying either the position of one of the colloids or the temperature. By subtracting the pairwise forces from the total force we are able to determine the many-body forces acting on one of the colloids. We have found that the many-body contribution to the total critical Casimir force is more pronounced for small colloid-colloid and colloid-substrate distances, as well as for temperatures close to criticality, where the many-body contribution to the total force can reach up to 25%.

CPP 20.2 Tue 18:15 Poster C

Viscosity of polyelectrolyte solutions and nanoparticle suspensions measured by AFM cantilevers — ●CAGRI ÜZÜM, ALEXANDRA ABRAHAM, HOWARD SETYAMUKTI, and REGINE VON KLITZING — Stranski-Laboratorium, Institut für Chemie, TU Berlin, Strasse des 17. Juni 124, 10623 Berlin, Germany

Density and viscosity of fluids can be determined locally i.e. in micro-scale using the frequency response of atomic force microscopy (AFM) cantilevers [1]. This contribution aims to measure the viscosity of polyelectrolyte solutions and nanoparticle suspensions at interfaces and at various volume scales. The interfacial viscosity can be manipulated by modifying the surface of the AFM cantilever (charge, hydrophobicity, etc.). The volume of interest can be controlled by tuning the resonance amplitude of the cantilevers via magnetic excitation [2]. In general, the viscosity of flexible polyelectrolyte (NaPSS, PAMPS) or small (9nm) particle systems measured by AFM increases with resonance amplitude and approaches the bulk viscosity. On the contrary, rigid polyelectrolyte (DNA, Chitin) or larger particle (26nm) systems have a significantly reduced micro-scale viscosity as compared to bulk. The entropic and kinetic sources of this difference will be addressed.

[1] Boskovic, S. et al. *J. Rheol.*, 2002, 46, 891-899

[2] McLoughlin, N. et al. *Appl. Phys. Lett.*, 2006, 89

CPP 20.3 Tue 18:15 Poster C

Dielectric spectroscopy of spherical Water/AOT/Decane microemulsions in the GHz regime — ●BJÖRN KUTTICH, ROBERT WIPF, and BERND STÜHN — Experimental Condensed Matter Physics, TU Darmstadt, Germany

Microemulsions are widely used ternary mixtures in industrial as well as fundamental research. Besides structural properties like the temperature depending shape and size of the microstructure, the dynamics of the microemulsions, especially in the spherical phase are of great interest. Focusing on spherical microemulsions in particular it is possible to change the properties of the existing surfactant shell by adding e.g. polymers either to the core or the matrix phase of the system. Investigating such polymer loaded spherical microemulsions slid into focus of recent research because they can be considered a model systems for the interaction between proteins and cell membranes.

Broadband dielectric spectroscopy is a commonly used method to investigate the dynamics of microemulsions. Using AOT based water in oil microemulsions it is possible to observe in addition to an enormous temperature dependency of the conductivity due to dynamic percolation also dielectric relaxations. The shell relaxation resulting from ion reorganisation in the surfactant shell evolves to the so called cluster relaxation while approaching the percolation temperature, which in turn can be influenced by adding different polymers. Following this relaxation up to the GHz regime allows now to investigate closer the formation of clusters during the percolation process.

CPP 20.4 Tue 18:15 Poster C

Temperature dependent behaviour of droplet and droplet shell in decan/AOT/H₂O microemulsions — ●MARKUS DOMSCHKE, SABINE BEST, and RUDOLF FEILE — TU Darmstadt, Institut für Festkörperphysik, Hochschulstraße 8, 64289 Darmstadt, Germany

The behaviour of water/AOT/decan microemulsions in the droplet phase of different sizes ($\omega = 2 - 40$) and droplet volume fractions of $\phi = 0.1 - 0.4$ is studied in a wide temperature range.

Combining differential scanning calorimetry (DSC) and refractive index measurements induce a new perspective of AOT-bound water in the droplets [1]. Small angle X-Ray scattering (SAXS) allows continuous analysis of the droplet structure between supercooling temperature of bulk water and phase separation temperature within a unique model. We introduce a combined structure factor of hard spheres [2] and *Ornstein-Zernicke* type [3].

[1] M. van Dijk *et al.*, *J. Phys. Chem.* **93**, 2506 (1989)

[2] N. W. Ashcroft and J. Lekner, *Phys. Rev.* **145**, 83 (1966)

[3] M. Kotlarchyk *et al.*, *Phys. Rev. A* **28**, 508- (1983)

CPP 20.5 Tue 18:15 Poster C

Vibrational density of states and molecular dynamics of discotic liquid crystals in the bulk and in the nanoconfined state investigated by neutron scattering — ●CHRISTINA KRAUSE¹, BERNHARD FRICK², REINER ZORN³, and ANDREAS SCHÖNHALS¹ — ¹BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany — ²Institut Laue Langevin, 6, rue Jules Horowitz, B.P. 156, F-38042 Grenoble Cedex 9, France — ³Juelich Centre for Neutron Science, Forschungszentrum Juelich, 52425 Juelich, Germany

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

CPP 20.6 Tue 18:15 Poster C

Micro-fabricated ionic liquid colloid emitter based on SU-8 capillaries with electroplated front electrodes — ●KATHARINA HUHN, MARKUS PIECHOTKA, TORSTEN HENNING, and PETER J. KLAR — Justus-Liebig-Universität, I. Physikalisches Institut, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

We manufactured a colloid emitter device using the negative resist SU-8 with multiple step photolithography. In the first step thin capillaries were manufactured with an inner diameter varying between 10 to 100 microns whilst the height is about 40 microns. In the second step a spacer layer was patterned. A metal grid structure was deposited onto the top of the surface of the spacer layer using evaporation, electroplating as well as ion beam etching. Afterwards the substrate was removed by wet chemical etching. For testing the device was bonded on a tank filled with an ionic liquid. An electric field was applied between the ionic liquid and the extraction electrode by using a high voltage source. The electro-spray emission was observed via videoscapy. We investigated the influence of different ionic liquids and capillary diameters on the required extraction voltage.

CPP 20.7 Tue 18:15 Poster C

Pressure calculation for polydisperse magnetic fluids — ●ELENA MININA^{1,2}, EKATERINA NOVAK¹, and SOFIA KANTOROVICH^{1,3} — ¹Ural Federal University, Lenin av. 51, Ekaterinburg, 620000, Russia — ²Institute for Computational Physics, University of Stuttgart, Allmandring 3, 70569, Stuttgart, Germany — ³Sapienza University of Rome, Piazzale A. Moro 5, 00185, Rome, Italy

Magnetic fluids (the systems of magnetic dipolar particles suspended in nonmagnetic liquids) possess a wide range of physical properties

which are currently under study. Typically, the synthesis of industrial magnetic fluids leads to a broad particle size distribution or so-called polydispersity of the system. Even in the absence of an external magnetic field the polydispersity plays a crucial role in cluster formation and significantly changes the microstructure of magnetic fluids what is confirmed by the work [C. Holm et al., *J. Phys.: Cond. Mat.* 18 (2006)]. In the present study we would like to elucidate how polydispersity influences one of the experimentally measurable macroscopic properties such as pressure of the system. We consider bidisperse system of magnetic dipolar soft or hard particles as the simplest case of polydisperse magnetic fluid. For such system we perform theoretical calculation of pressure using method of diagram expansion that is in a good agreement with data obtained via molecular dynamics simulations in ESPResSo. The final analysis of pressure for bidisperse system confirms that the pressure is very sensitive to the polydispersity of the system.

CPP 20.8 Tue 18:15 Poster C

The Effect of Different Polymer Length on Water Droplets of Reverse AOT microemulsion — ●MASOUD AMIRKHANI¹, SOHEIL SHARIFI¹, SÉRGIO FUNARI², and OTHMAR MARTI¹ — ¹Institut für Experimentelle Physik, Universität Ulm, Albert-Einstein-Allee 11 89081 Ulm — ²HASYLAB, Notkestrasse 85, D-22607 Hamburg, Germany

We study the effect of polyethylene glycol (PEG) on the dynamic and structure of the reverse AOT microemulsion. The mixture of water and oil with anionic surfactant AOT (sodium bis-(2-ethylhexyl) sulfosuccinate) can form microemulsion. The dynamic of microemulsion in the presence of PEG is investigated by photon correlation spectroscopy technique. We mainly focus on the variation of the translational diffusion behavior as a function of the polymer concentration and polymer length scale. By increasing the content of the lowest PEG length scale ($M_n=285$) the dynamic of microemulsion slows down. In addition, one relaxation process is distinguished for all polymer concentration. However, for the two higher polymer length scale ($M_n=2200$ and 6000) two relaxations are observed and the dynamic of microemulsion speed up. We used the small angle X-ray scattering technique to monitor the size and the polydispersity of the mixture system (AOT-microemulsion/PEG).

CPP 20.9 Tue 18:15 Poster C

A multicolor interferometer for the simultaneous measurement of contrast factors — ●THOMAS TRILLER and WERNER KÖHLER — Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany

During the last years thermodiffusion in ternary fluid mixtures has been the subject of gaining interest. Currently, optical experiments are performed both in a microgravity environment on board of the international space station (ISS) using an interferometric device (SODI) and on ground using the beamdeflection technique [1]. These experiments make use of a change in the refractive index n to analyse changes in the concentration of the mixtures. To interpret the data, a precise knowledge of the so called contrast factors $(\partial n/\partial c_i)_{p,T,c_j \neq i}$ and $(\partial n/\partial T)_{p,c_i}$ is essential. Monte Carlo simulations have shown that errors in the refractive index need to be as low as 10^{-5} to get reliable values for the Soret coefficients. As a step to reach such precision, we present a new setup capable of measuring contrast factors at five different wavelengths simultaneously. The basic outline consists of a Michelson-Interferometer with a special sample cell.

[1] Königer, A., Wunderlich, H. and Köhler, W., *J. Chem. Phys.* **132**, pp. 174506, 2010.

CPP 20.10 Tue 18:15 Poster C

Self assembly in a two-dimensional system of hard disks with quadrupolar interaction — ●MALTE KÄHNE and SABINE H. L. KLAPP — Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

Using standard Monte Carlo algorithms in the grand canonical ensemble, we examine the thermodynamic properties and the structural behaviour of a two-dimensional hard disk fluid with quadrupolar interaction potential. At low temperatures, this liquid exhibits a cluster phase. We locate this cluster phase and study the aggregation of these clusters as well as their size distribution. We analyse the structure of these clusters by local bond-angle order parameters and the pair correlation function. Our results illustrate the likelihood of the T-structure, which is also found as a stable crystal structure for three-dimensional quadrupolar fluids [1].

[1] C. Vega, B. Garzon, S. Lago and P. A. Monson, *J. Mol. Liq.* **73**, 157 (1998)

CPP 20.11 Tue 18:15 Poster C

Network formation in polydisperse colloidal systems induced by an uni-axial external field — HEIKO SCHMIDLE, SEBASTIAN JÄGER, ●FLORIAN KOGLER, and SABINE H.L. KLAPP — Institut für Theoretische Physik, TU Berlin, Hardenbergstr. 36, D-10632 Berlin, Germany

Using Molecular Dynamics and Monte Carlo simulations we investigate a theoretical model of two-dimensional colloids with one or two (anti-parallel orientated) induced dipole moments mimicking recent experiments on mixtures of polystyrene colloids with and without gold patches in the presence of an external electric field [1]. Such systems percolate in field direction and perpendicular to it. We are able to determine percolation transitions for both cases and identify basic connection types of different colloids [2]. Furthermore the percolated model system shows strongly hindered translational dynamics indicating gelation.

[1] S. Gangwa, A. Pawar, I. Kretzschmarb and O. D. Velev, *Soft Matter*, 6:1413-1418 (2010)

[2] H. Schmidle, S. Jäger, C. K. Hall, O. D. Velev, and S. H. L. Klapp, Two-dimensional colloidal networks induced by a uni-axial external field, submitted (2012)

CPP 20.12 Tue 18:15 Poster C

Magnetic Field Controlled Composite Paramagnetic-Diamagnetic Colloidal Phases — ●FABIAN WAGLE, AYAN RAY, and THOMAS FISCHER — EPV, Uni Bayreuth

We report on differently ordered colloidal phases of a mixture of paramagnetic and diamagnetic colloids subject to a quickly varying time dependent magnetic field. Effectively paramagnetic and effectively diamagnetic colloids are created from paramagnetic and nonmagnetic colloids immersed into a thin film of aqueous ferrofluid. The time-averaged dipole interaction between induced dipoles can be characterized by a uniaxial external precession angle and a biaxial eccentricity characterizing the anisotropy of the external field modulation. The variation of both control parameters causes a sequence of transitions between differently correlated orientation order between the paramagnetic and diamagnetic colloids. We observe the formation of bonds between paramagnets and diamagnets along one or two directions with a staggered order of the magnetic moments. Bonds between similar particles with uniform order of the magnetic moments form along directions orthogonal to bonds between different particles along the staggered directions. When the external precession angle passes the magic angle, the particle order rearranges and staggered directions with bonds between different particles change into uniformly ordered directions with bonds between similar particles and vice versa. The transition in order occurs in two steps with a biaxial phase intervening between the two uniaxial ordering phases.

CPP 20.13 Tue 18:15 Poster C

Noninvasive measurement of dissipation in colloidal systems — ●JAKOB MEHL¹, BORIS LANDER², UDO SEIFERT², and CLEMENS BECHINGER^{1,3} — ¹2. Physikalisches Institut, Universität Stuttgart, Germany — ²II. Institut für Theoretische Physik, Universität Stuttgart, Germany — ³Max-Planck-Institute for Intelligent Systems, Stuttgart, Germany

According to Harada and Sasa [*Phys. Rev. Lett.* 95, 130602 (2005)], heat production generated in a nonequilibrium steady state can be inferred from measuring response and correlation functions. In many colloidal systems, however, it is a nontrivial task to determine response functions, whereas details about spatial steady state trajectories are easily accessible. Using a simple conditional averaging procedure, we show how this fact can be exploited to reliably evaluate average heat production. By combining paramagnetic colloidal particles, rotating laser tweezers and digital video microscopy, we apply the new method to two nonequilibrium steady states, which can be coupled by an externally controlled magnetic field. We show, that the average heat production is nonmonotonic in the coupling strength and even for low statistics quite robust results are available [*Phys. Rev. E.* 86, 030401(R) (2012)].

CPP 20.14 Tue 18:15 Poster C

Structure of confined microemulsions in AAO nanopores — ●FREDERIK LIPPERT and HENRICH FRIELINGHAUS — Jülich Centre for Neutron Science, Forschungszentrum Jülich GmbH, 85747 Garching

Microemulsions are used in a variety of different applications such as detergency or oil recovery where they are exposed to a variety of surfaces and confinements. We analyzed the structure of symmetrical microemulsions with different surfactant concentrations in two-dimensional confinement using cylindrical nano pores arranged hexagonally on anodized aluminum oxide (AAO) membranes. The microemulsions we used have a water-oil domain sizes in the range of 200Å while the pores we used have diameters of 180nm and 400nm. We found the microemulsion exhibiting a lamellar, shell-like structure at the interface even though their equilibrium state is bicontinuous. We used small angle neutron scattering for the analysis because of the neutron wavelength being comparable to the examined structures and the possibility of contrast matching the microemulsion to the AAO membranes by partly replacing the H₂O with D₂O. This matching suppresses the scattering from the membrane which would overshadow the scattering from the microemulsion and makes the microemulsion scattering accessible. The scattering from the interface near lamellar structure is Bragg like while the scattering from the bicontinuous microemulsion in the pore center is isotropic. Both structures have the same domain size so in order to distinguish between both structures we set up the sample perpendicular to the incoming neutron beam then turned it 15° making the scattering from the lamellar structure visible.

CPP 20.15 Tue 18:15 Poster C

Directional locking and dynamical ordering of fluid colloidal monolayers driven across quasiperiodic substrate potentials — ●THOMAS BOHLEIN, CHRISTOPH JULY, and CLEMENS BECHINGER — 2. Physikalisches Institut, Universität Stuttgart, Germany

Particles driven across an ordered potential energy surface may either follow the direction of the driving force or become entrained along any of the commensurate directions of the substrate. Such directional locking effects are of great technological relevance since they allow sorting of particles according to their size or refractive index. Here we experimentally study the sliding behavior of a two dimensional disordered colloidal monolayer interacting with quasiperiodic light induced substrate potentials. When the direction of the driving is varied with respect to the substrate, we find directional locking at angles corresponding to the symmetry axes of the underlying potential. On the locking steps the colloids assemble into dynamically ordered structures which consist of periodically spaced bands. We show that such ordered colloidal phases can be understood within the framework of periodic average structures which stems from the structure determination of complex metal alloys.

CPP 20.16 Tue 18:15 Poster C

Fundamental mixed measure theory for fluids of hard particles — ●RENÉ WITTMANN and KLAUS MECKE — Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany

A density functional for anisotropic hard bodies can be constructed in terms of weighted densities which depend on geometry and position of only one single oriented particle [1]. We study the liquid crystalline behavior of a system of hard spherocylinders and compare the results to Monte-Carlo simulations.

The density profile and the director dependence at the isotropic-nematic interface show the correct behavior. The functional also provides closed formulas for the Frank elastic coefficients via the Poniewierski-Stecki equations. The original fundamental measure theory is improved by eliminating the divergence in the free energy of the otherwise unstable smectic phase.

We propose a new geometric method to derive the low-density limit of the exact density functional. Here, so-called mixed measures of two bodies are used rather than weighted densities of only one single particle. This might evade present approximations and lead to an improved density functional for liquid crystals.

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

CPP 20.17 Tue 18:15 Poster C

Measuring thermal diffusion of binary mixtures using a two color optical beam deflection technique — ●MATTHIAS GEBHARDT and WERNER KÖHLER — Physikalisches Institut, Universität Bayreuth, D-95440 Bayreuth, Germany

We have measured and analyzed in detail the Soret, diffusion and thermal diffusion coefficients of the binary mixtures of dodecane, isobutylbenzene and 1,2,3,4-tetrahydronaphthalene, the benchmark systems

that are currently also investigated on board the International Space Station ISS in the DCMIX program, at various concentrations. The measurements were performed using a two color optical beam deflection technique, which is equipped with two laser diodes one at 405nm and the other at 635nm. With these two wavelengths we can measure one sample and receive simultaneously two deflection signals. The two signals can be used independently to evaluate the transport coefficients in order to verify the results. The measured beam deflection signal is strongly determined by the so called contrast factors. These contrast factors are the derivatives of the refractive index with respect to concentration and temperature, which have to be determined with high accuracy. We use the Lorentz-Lorenz equation and also the modified equation by Looyenga, to calculate the contrast factors using the refractive index, density and molecular polarizability, as described by Li et al [1]. In order to obtain a quantitative agreement with the experimental data, it is necessary to take the temperature dependence of the molecular polarizabilities into account.

[1] W. B. Li et al., The Journal of Chemical Physics 101, 5058 (1994)

CPP 20.18 Tue 18:15 Poster C

Particle dynamics in dense suspensions flowing through microchannels — ●MICHEL DUITS — MESA+ Institute, University of Twente, PO Box 217, 7500 AE Enschede, The Netherlands

We will report on a systematic study, aimed at understanding the dynamics of colloidal hard spheres inside microfluidic channels. Real-time confocal microscopy is used to visualize the structure, diffusion and flow of model suspensions of 1 micron diameter silica spheres. By controlling the flow speed, we cover a range of Peclet numbers ($\ll 1$ and $\gg 1$) so we can study both the diffusion-controlled and the flow-controlled dynamics. Analysis of the apparent diffusion coefficient in the direction perpendicular to the flow reveals a clear spatial dependence of the diffusivity on the distance to the wall(s). While this is found both at low and at high Peclet numbers, the manifestations and underlying mechanisms are very different.

CPP 20.19 Tue 18:15 Poster C

Influence of molecular structure on rheological properties of hydrogen bonded supramolecular polymeric melts — ●TINGZI YAN¹, KLAUS SCHRÖTER¹, FLORIAN HERBST², WOLFGANG BINDER², and THOMAS THURN-ALBRECHT¹ — ¹Institute of Physics, Martin-Luther University Halle-Wittenberg, Halle 06120, Germany, — ²Institute of Chemistry, Martin-Luther University Halle-Wittenberg, Halle 06120, Germany,

Combining SAXS and rheology the relation between self-assembly and mechanical properties has been studied. A semi-quantitative understanding of the influence of structure on the rheological properties in the bulk state has been achieved. Three polyisobutylene samples with thymine/2,6-diaminotriazine functional end groups were used as model system. Two different solidification scenarios were observed. In one case ordering of micelles at lower temperatures can be observed. In the second case the formation of disordered hydrogen bonded network leads to gelation at lower temperatures.

CPP 20.20 Tue 18:15 Poster C

Friction of colloidal monolayers on a periodic substrate — ●CHRISTOPH JULY, THOMAS BOHLEIN, and CLEMENS BECHINGER — 2. physikalisches Institut, Universität Stuttgart

Friction is an ubiquitous and fundamental phenomenon in our every day life. While its precise control is highly desirable for technical applications, a comprehensive understanding of friction is still lacking. On the macroscopic level asperities mediate a partial contact between two surfaces leading to the well known static and dynamic friction. However, many interesting friction effects only happen on an atomic scale. Friction phenomena of sliding atomic monolayers in this regime are theoretically described by the Frenkel-Kontrova model. One particular effect, that is predicted by this theory, is the so called Aubry-Transition. This transition gives rise to a jump from static friction to a superlubric state (frictionless) between two incommensurate monolayers as the interaction between the atoms of a single monolayer grows in strength and exceeds a critical value. Yet systems of nano meter size are very hard to observe experimentally. To overcome this difficulty we devised a colloidal model system to emulate the nanoscopic world, enabling us to measure nano tribologic effects with microscopic particles. For this purpose we employ para-magnetic particles, which allow us to tune the particle-particle interaction by applying an external magnetic field. Monolayers of these particles are situated on a potential landscape generated by a light field and pulled across this

periodic substrate. In doing so, we are able to directly observe the Aubry transition for the first time.

CPP 20.21 Tue 18:15 Poster C

Gradient diffusion in mono- and bidisperse magnetic fluids — ●ALLA MURATOVA¹, ALEXEY IVANOV¹, and SOFIA KANTOROVICH^{1,2} — ¹Ural Federal University, Lenin av. 51, 620000, Ekaterinburg, Russia — ²Sapienza, University of Rome, Piazza A. Moro 5, 00185, Rome, Italy

We present the results on the mobility and diffusion coefficients in the systems of magnetic dipolar particles. In our study we firstly investigate the influence of chain formation and polydispersity of particles on self-diffusion. Here, we use Density Functional Approach and direct calculations to elucidate why the formation of chains leads to the average decrease of mobility in monodisperse systems, but in the case of a bidisperse particle size distribution the particle mobility becomes a function of the fractional composition. As the second step we calculate the diffusion coefficients using the mobility coefficients obtained before for both mono- and bidisperse systems of magnetic particles. Here, we mainly focus on the diffusion induced by the gradient of the total ferroparticle density. Finally, we use the diffusion coefficients to calculate the distribution of chains in the gravity gradient. We extensively compare our results to the simulation data and find them in a good agreement.

CPP 20.22 Tue 18:15 Poster C

Synthesis of Hematite particles monitored using in-situ SAXS and WAXS — ●ALEXANDER SCHAVKAN, FABIAN WESTERMEIER, INGO STEINKE, JAN PERLICH, BIRGIT FISCHER, GERHARD GRÜBEL, and MICHAEL SPRUNG — DESY Deutsches Elektronen-Synchrotron, Notkestraße 8, 22607 Hamburg, Deutschland

To study the statistical physics of phase transitions, colloidal suspensions are often used as model systems. Due to their complex phase diagrams, suspensions of anisotropic nanoparticles, like hematite particles, are particularly interesting. These particles can be synthesized with varying size aspect ratios and can be aligned in an external magnetic field. The described experiments aimed to investigate the evolution of the synthesis and the appearance and growth of the magnetic moment during the chemical reaction.

Two syntheses were performed under an applied static magnetic field and monitored using in-situ SAXS and WAXS. While in one of these syntheses the growth of anisotropic, spindle shaped particles was induced by the addition of NaH₂PO₄, the second chemical reaction yielded isotropic, cubic shaped particles. By SAXS measurements the appearance of a magnetic moment in the particles and the development of the particle size and size distribution was investigated. WAXS experiment monitored the change in the chemical composition of the particles from Iron(III)chloride to hematite (β -Iron(III)oxide).

This contribution shows the details and the results of the experiment.

CPP 20.23 Tue 18:15 Poster C

Interactions of colloids and DNA with confining charged nano-channels: Analysis of numerical solutions of the Poisson-Boltzmann equation and molecular dynamics simulations. — ●DMITRY ROZHKOV¹, ALEXANDER SCHLAICH², SOFIA KANTOROVICH^{1,3}, and MARCELLO SEGA⁴ — ¹Ural Federal University, Lenin av. 51, 620000, Ekaterinburg, Russia — ²Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin — ³Sapienza, University of Rome, Piazza A. Moro 5, 00185, Rome, Italy — ⁴Tor Vergata University of Rome, via della Ricerca scientifica 1, I-00133 Rome, Italy

Nanosopic confinement of ionic solutions is often met in both biological systems and technical applications but the computation of electrostatic interactions in electrolyte solutions is still challenging. The Poisson-Boltzmann equation can be used for the simple case of monovalent ions. The numerical solution usually implies that the boundary conditions are known a priori, but in strongly confined systems such as charged nano-channels or for strongly overlapping Debye-layers the usual assumptions of constant potential or constant flux boundary conditions break down. Molecular dynamics simulations proved to be an efficient tool to analyse systems with dielectric mismatch. However, realistic salt concentrations and confinements are rarely feasible in simulations. We use both a numerical Poisson-Boltzmann scheme and molecular dynamics simulations for calculating the effects of colloidal particles and DNA in confinement in order to elucidate the effect observed by Krishnan et al [Nano Lett., 7, 1270 (2007)].

CPP 20.24 Tue 18:15 Poster C

Controlling the cross-linker distribution and shell thickness of gold-poly-NIPAM core-shell colloids — ●MATTHIAS KARG¹, PAUL MULVANEY², SABINE ROSENFELDT³, and SARAH JABER² — ¹Universität Bayreuth, Physikalische Chemie - Kolloidale Systeme — ²University of Melbourne, School of Chemistry & Bio21 Institute — ³Universität Bayreuth, Physikalische Chemie I

The encapsulation of inorganic nanoparticles with responsive polymer networks has attracted significant interest in recent years, since such materials can combine properties of their different components. Most effort so far was devoted to the encapsulation of different inorganic cores such as silica, gold and silver nanoparticles. It has been demonstrated that cores with a broad range of sizes can be used to build up such core-shell colloids. The present contribution focuses on the control of the polymer network structure rather than on the nanoparticle core. We encapsulated 15 nm gold nanoparticles into thermoresponsive polymer shells composed of NIPAM with a constant feeding of the cross-linker BIS during the polymerization. This leads to core-shell colloids with single nanoparticle cores well encapsulated in homogeneously cross-linked poly-NIPAM shells. Additional polymerization steps can be used to overgrow the shells still keeping the cross-linker distribution homogeneous. Analysis using TEM, AFM and UV-Vis-spectroscopy will be presented. The shell morphology was investigated with SANS. An Ornstein-Zernicke analysis of the scattering profiles clearly reveals a homogenous network structure with correlation lengths of approx. 1.5 nm.

CPP 20.25 Tue 18:15 Poster C

Sedimentation and orientational order of active bottom-heavy particles — ●KATRIN WOLFF, MARC HENNES, and HOLGER STARK — Institut für Theoretische Physik, Technische Universität Berlin

Self-propelled particles in an external gravitational field have been shown to display both an increased sedimentation length and polar order even without particle interactions [1,2]. Here, we investigate self-propelled particles which additionally are bottom-heavy, that is they feel a torque aligning them to swim against the gravitational field. We study their dynamics in an external gravitational field analytically and numerically using Brownian dynamics simulations. For bottom-heavy particles the gravitational field has the two opposite effects of i) sedimentation and ii) upward alignment of the particles' swimming direction. Depending on the strength of gravity, the particles' swimming speed and the aligning torque, we observe either effective sedimentation with increased sedimentation length (compared with the passive case but also the active case without bottom-heaviness) or inversion where particles swim towards the top of the box. We will give analytical results for sedimentation lengths and polar order in the dilute limit and numerical results for the case with hydrodynamic interactions where particles form vortices and columns.

[1] J. Palacci et al., Phys. Rev. Lett. 105, 088304 (2010)

[2] M. Enculescu and H. Stark, Phys. Rev. Lett. 107, 058301 (2011)

CPP 20.26 Tue 18:15 Poster C

Clustering and chemotactic collapse in a system of self-phoretic active particles — ●OLIVER POHL and HOLGER STARK — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin, Germany

Recent experiments of active colloids show a coexistence of single particles and clusters [1]. In such a "hot-cluster state" the clusters are themselves active and their sizes vary in time. In our model we separate two phoretic effects where the first accounts for activity and the second for interactions between the particles. Each colloid produces a gradient of a chemical which generates phoretic motion of nearby colloids; similar to bacteria moving along gradients of chemicals.

A hot-cluster state is reproduced which, depending on two parameters controlling interaction and activity, may exhibit a collapse to a single-cluster state. Such a collapse as well as the hot-cluster state have experimentally been observed in colonies of self-propelling bacteria [2,3]. The hot-cluster state is characterized by a power-law cluster distribution. Using a theory for nucleation and growth of clusters, we explain how clustering initiated by chemotaxis may be distinguished from clustering of particles with purely steric interactions.

[1] I. Theurkauff, C. Cottin-Bizonne, J. Palacci, C. Ybert, and L. Bocquet, Phys. Rev. Lett. 108, 268303 (2012).

[2] F. Peruani, J. Starrus, V. Jakovljevic, L. Søgaard-Andersen, A. Deutsch, and M. Bär, Phys. Rev. Lett. 108, 098102 (2012).

[3] E. Budrene, and H. Berg, *Nature* **349**, 630 (1991).

CPP 20.27 Tue 18:15 Poster C

Immunoglobulin G in Solution with Polyethylene Glycol: Protein Interaction and Phase Transitions — ●BO JING¹, ANASTASIA DIETRICH¹, SALIBA BARSAUME¹, FAJUN ZHANG¹, MICHAEL SZTUCKI², and FRANK SCHREIBER¹ — ¹Institute of Applied Physics, University of Tübingen — ²ESRF, Grenoble, France

Immunoglobulin G (IgG) plays a crucial role in the immune response by interacting with the proteins of pathogens. In addition, the interaction of IgG with itself and the resulting liquid-liquid phase separation (LLPS) or crystallization is also of great interest, e.g. for the understanding of cryoglobulinemia and for pharmaceutical applications. In these cases, it is desirable to control the phase behaviour of IgG in solution. We achieve this through the addition of polyethylene glycol (PEG) to bovine plasma IgG solutions, which allows us to tune the range and strength of short-range attractive interactions between IgG molecules. We measured the IgG PEG solutions by small-angle X-ray scattering (SAXS) and we observed a significant dependence of the interaction on IgG concentration, PEG molecular weight and concentration as well as temperature. The two-Yukawa potential is used to fit our data, and the so obtained potential parameters are associated with the detailed phase diagrams which we compiled over the same four parameters. Thereby, we identify quantitative conditions on the interaction potential under which phase transitions occur in IgG PEG solutions. These findings allow us to assess the significance of specific, anisotropic interactions between IgG molecules in the explanation of the observed SAXS data and macroscopic phase behaviour.

CPP 20.28 Tue 18:15 Poster C

On the Formation of Clusters in Protein Solutions Upon Addition of Multivalent Ions — ●DANIEL SORARUF¹, FAJUN ZHANG¹, FELIX ROOSEN-RUNGE¹, TILO SEYDEL¹, RALF SCHWEINS², and FRANK SCHREIBER² — ¹Institut für Angewandte Physik, Tübingen — ²ILL, Grenoble, France

Formation of clusters of proteins in solution are currently of strong fundamental interest, and also of enormous practical interest, from amyloidogenic diseases to food and pharma industry. Current research focuses on the mechanism of protein clustering, its role in phase transitions, the lifetime and stability of clusters. We investigate protein solutions of bovine serum albumin (BSA) with YCl_3 . The system exhibits a reentrant transition, characterized by the boundaries c^* and c^{**} for the concentration of Y^{3+} ions; in between the system is in a condensed regime[1]. We study the formation of clusters approaching c^* by means of SLS/DLS, obtaining information about diffusion coefficient, compressibility, and size of the clusters[2]. A continuous decrease in diffusion coefficient and increase in overall scattered intensity reveal the formation of aggregates of 100 nm in solution, which are stable over days. The inverse forward scattering intensity decreases linearly over a broad salt concentration range and the compressibility diverges close to c^* . Results from different protein concentrations can be rescaled into a master curve as a function of normalized c_{salt}/c^* . The formation of the clusters could be related to charge balance and patchy attraction of the proteins. [1] F. Zhang et al., *PRL* **101**, 2008, 148101; [2] Roosen-Runge et al., *PNAS* **108**, 2012, 11815.

CPP 20.29 Tue 18:15 Poster C

Phase separation patterns in colloidal suspensions of anisotropic pigment particles — ●KATHRIN MAY, ALEXEY EREMIN, and RALF STANNARIUS — Institute of Experimental Physics, Faculty for Natural Science, Otto von Guericke University Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

The physics of colloidal suspensions of anisotropic particles has been a topic of research since almost a decade now. Such suspensions show a variety of unique properties depending on the particle concentration and on external fields. Here, we report the relaxation of electric-field-induced inhomogeneities in particle concentration. The occurring patterns can be static or dynamic. For our experiments, we use electro-responsive suspensions of pigment particles 'Novoperm Carmine HF3C' (Clariant) with an aspect ratio of about 1:5 in a non-polar solvent.

CPP 20.30 Tue 18:15 Poster C

Mechanical load on colloidal and granular systems observed by fast confocal microscopy — ●GÜNTER K. AUERNHAMMER, MARCEL ROTH, MANOS ANYFANTAKIS, JENNIFER WENZL, and HANS-JÜRGEN BUTT — Max-Planck-Institut für Polymerforschung, Mainz,

Germany

Densely packed colloidal and granular systems under mechanical load may show significant internal reorganization on a microscopy level. On a macroscopic level these reorganizations lead to permanent (plastic) deformations of the sample even at vanishing deformations of the colloids or granulates [1,2]. We use a combination of fast confocal microscopy (frame rate up to 500 Hz) [3] and nano indentation to explore the influence of a finite speed of the deformation on the reorganization dynamics. We also address specific changes that arise when switching from deformation controlled to stress controlled experiments.

[1] M. Roth, C. Schilde, Ph. Lellig, A. Kwade, G. K. Auernhammer, *Eur. Phys. J. E* **35** (2012) DOI 10.1140/epje/i2012-12124-8.

[2] M. Roth, C. Schilde, Ph. Lellig, A. Kwade, G. K. Auernhammer, *Chem. Lett.* **41** (10), 1110-1112 (2012).

[3] G. K. Auernhammer, M. Roth, and H.-J. Butt, Patent DE-10 2012 101 344.6

CPP 20.31 Tue 18:15 Poster C

Wettability controlled transfer of colloidal assemblies from wrinkled elastomers — CHRISTOPH HANSKE¹, ●MAREEN MÜLLER¹, VERA BIBBER¹, MORITZ TEBBE¹, SARAH JESSL¹, ALEXANDER WITTEMANN², and ANDREAS FERY¹ — ¹University of Bayreuth, Germany — ²University of Konstanz, Germany

Assemblies of nanoparticles are promising building blocks for future sensoric devices. Highly ordered arrays of nanoparticles can be realized by convective assembly on surface-wrinkled elastomers.[1] Recently, this lithography-free procedure was developed further to allow subsequent particle transfer to solid substrates, which is a prerequisite for many technological applications.[2] Compatibility with a variety of functional particles was also demonstrated. In this contribution we discuss the roles of capillary forces and surface wettability for the wet transfer of colloidal assemblies. In contrast to adhesion-based printing or lift-off methods, conformal contact between the particles and the target substrate is not required. However, successful particle transfer depends on the wettability of the target substrate and is inhibited efficiently by a hydrophobic monolayer.[3] We demonstrate that chemically patterned substrates are sufficient to control the particle transfer locally with excellent precision. Our method is robust enough to conduct multiple deposition steps, resulting in hierarchical colloidal structures with potential applications in plasmonic sensing or the construction of metamaterials. [1] C. Lu, et al., *Soft Matter* **2007**, **3**, 1530. [2] M. Müller, et al., *Nanoscale* **2012**, **4**, 2491. [3] C. Hanske, et al., *Langmuir* **2012**. 10.1021/la304028f

CPP 20.32 Tue 18:15 Poster C

Hydrodynamic dispersion of micron-sized colloids in micro structured porous media — ●FRANK WIRNER¹, CHRISTIAN SCHOLZ¹, and CLEMENS BECHINGER^{1,2} — ¹2. Physikalisches Institut, Universität Stuttgart, Germany — ²Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany

Hydrodynamic dispersion of solutes and colloids in porous media occurs under the combined actions of a spatially varying velocity field that is caused by the morphology of the porous matrix and molecular diffusion. This spreading apart of initially adjacent colloids is important to a wide variety of processes such as secondary oil recovery, groundwater pollution or blood perfusion inside the body.

We study the dispersion of diluted suspensions of micron-sized colloids in quasi-2D microporous structures, created using soft lithography, over a wide range of Péclet numbers and porosities. A camera system is used to track individual particles and analyze their trajectories. From the obtained trajectories we calculate the velocity field of the particles and determine the first-passage-time distributions that in turn are related to the dispersion coefficients. 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 the first-passage-time distributions. We discuss the effects that lead to long-tailed distributions.

CPP 20.33 Tue 18:15 Poster C

Positron annihilation lifetime spectroscopy in a porous liquid — ●TÖNJES KOSCHINE¹, KLAUS RÄTZKE¹, NICOLA GIRI², and STUART L. JAMES² — ¹Christian-Albrechts-Universität Kiel, Institute for Material Science - Multicomponent Materials, Kaiserstraße 2, Kiel, Germany — ²School of Chemistry and Chemical Engineering, Queen's University Belfast, Stranmilis Road, Belfast, Northern Ireland

Porous liquids (PL), or liquids with intrinsic porosity, are a new type

of material [1]. In contrast to well known cavities between molecules of a liquid (extrinsic porosity), intrinsic porosity refers to empty voids within the molecules. The materials are composed of rigid cages to which short hydrocarbon tails or cyclic crown ethers are attached to endow liquid-like behavior, or very high solubility in liquid crown ether solvents respectively. The main question is whether such side groups or solvent molecules remain outside the cage cavities or whether they are able to occupy the cage cavities over time. Positron annihilation lifetime spectroscopy (PALS) is a suitable tool to detect empty pores in the sub-nanometer range. The measured orthopositronium lifetime is directly related to the pore size by the Tao-Eldrup model. Two different series of PL were studied at various temperatures by PALS to find evidence for permanent intrinsic porosity. A detailed analysis of the spectra as function of temperature, involving both PL and control materials, allowed clear separation of the lifetime due to the side groups and lifetime due to the empty pores in the PL. Thus, we were able to prove that the pores in these liquids are indeed permanently empty.

[1] O Reilly, N.; Giri, N.; James, S.L.: Chem. Eur. J., 13, 2007, 3020-3025.

CPP 20.34 Tue 18:15 Poster C

The effect of topology on the conformations of cyclic polymers in melts — •MICHAEL LANG¹, JAKOB FISCHER^{1,2}, and JENS-UWE SOMMER^{1,2} — ¹Leibniz Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden — ²Institut für Theoretische Physik, Technische Universität Dresden, 01069 Dresden

The bond fluctuation method is used to simulate solutions and melts of entangled and interpenetrating cyclic polymers. The swelling of interpenetrating rings upon dilution follows the same laws as for linear chains. We find an exponential decay of the knotting probability of cyclic polymers as function of the number of blobs per chain. A power law dependence $f_n \sim \phi R^2 \sim \phi^{0.77} N$ for the average number f_n of linked rings of N monomers per cyclic polymer at polymer volume fractions ϕ larger than the overlap volume fraction of rings ϕ^* is determined from the simulation data. The fraction of non-concatenated cyclic polymers displays an exponential decay $P_{OO} \sim \exp(-f_n)$, which indicates f_n to provide the entropic effort for not forming concatenated conformations. These observations indicate four different regimes for the conformations of cyclic polymers in melts separated by characteristic lengths N_{OO} , N_C and N^* that describe the onset of the effect of non-concatenation, the cross-over between weak and strong compression and the cross-over to an overlap dominated concatenation contribution respectively. In these regimes, ring size scales as N^α with $\alpha = 1/2, 2/5, 3/8$, and $4/9$ respectively. The available data is in agreement with the first three regimes. The last regime is still unconfirmed due to the extremely large N necessary to reach this regime.

CPP 20.35 Tue 18:15 Poster C

In-situ spray deposition of colloidal thin films - a mi-

crobeam GISAXS study — •STEPHAN VOLKHER ROTH¹, GUNTARD BENECKE^{1,2}, SEBASTIAN BOMMEL¹, BERIT HEIDMANN¹, GERD HERZOG¹, ROMAN MANNWEILER¹, JAN PERLICH¹, JOHANNES RISCH¹, GONZALO SANTORO¹, MATTHIAS SCHWARTZKOPF¹, SHUN YU¹, KUHUSARKAR³, and PETER MÜLLER-BUSCHBAUM³ — ¹DESY, Notkestraße 85, D-22607 Hamburg — ²MPI Coll. Inter. Golm, Abt. Biomat., Wissenschaftspark Potsdam-Golm, D-14424 Potsdam — ³Lehrst. funkt. Mat., TU München, James-Franck-Str. 1, D-85748 Garching

Fast, flexible and reliable production of thin films in organic photovoltaic devices has led to the use of fluid spray deposition as one method of choice [1,2]. This method is easy to employ while at the same time yielding fully functional devices with comparable efficiencies. Spray deposition is a complex fluidic process based on nanolitre droplets. To tailor the structure-function relationship starting from the nanoscopic level, it is therefore mandatory to understand the layer formation during the spraying process in-situ. We combined colloidal solution spraying and grazing incidence small-angle x-ray scattering in-situ to explore the rapid structural build-up during spraying as a function of different solvents and especially as a function of temperature. We present our results on this high-throughput combinatorial study and show that especially the latter parameter is crucial to obtain homogenous thin polymeric films. [1] Vak et al., Appl. Phys. Lett. 91, 081102 (2007) [2] Alaa et al., Adv. Funct. Mat. 22, 4078 (2012)

CPP 20.36 Tue 18:15 Poster C

Determining the shear viscosity of a solvent in the presence of electric fields — •ZORAN MILIČEVIĆ¹, DAVID M. SMITH², and ANA-SUNČANA SMITH¹ — ¹Institut für Theoretische Physik and Cluster of Excellence: Engineering of Advanced Materials, Universität Erlangen-Nürnberg, Erlangen, Germany — ²Computer Chemie Centrum, Universität Erlangen-Nürnberg, Erlangen, Germany

The shear viscosity is a very important kinetic property characterizing the macroscopic properties of molecular systems and is hence useful for the parametrization of reliable force fields. However, calculating the shear and bulk viscosities from molecular dynamics simulations is still a challenging task.

Here we study the shear viscosity of water by performing extensive MD simulations using the GROMACS software package and SPC/E model of water (rigid and flexible) as a function of the electric field strength. The latter breaks the otherwise isotropic nature of the solvent. The shear viscosity is related to the autocorrelation function of the off-diagonal elements of the pressure tensor by the Green-Kubo relation, which is used to analyze pure water simulations. Alternatively, the viscosity is calculated from the mobility of a spherical particle, the latter arising from the diffusion constant evaluated in independent simulations. Apart from the fact that different treatments show excellent agreement, we find that the field decreases the component of the shear viscosity perpendicular to the field and increases the components parallel to the field.

CPP 21: Transport: Molecular Electronics (joint session TT/CPP/HL/MA)

Time: Wednesday 9:30–12:45

Location: H2

CPP 21.1 Wed 9:30 H2

Inelastic scattering effects and electronic shot noise — •AMIN KARIMI, MARKUS HERZ, and ELKE SCHEER — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

The study of shot noise for junctions formed by single molecules offers interesting new information that cannot be easily obtained by other means. At low bias it allows determining the transmission probability and the number of current carrying conductance channels [1]. We investigate the effects of phonon scattering on the electronic current noise through nano junctions with mechanically controllable break junction (MCBJ). Equivalent measurements have recently been reported to be able to reveal inelastic transport contributions to the current through gold atomic contacts [2]. We developed a new and versatile measurement system enabling measurements of the noise in a rather broad range of conductance values from $0.01 G_0$ to $1 G_0$ without the necessity of double wiring. First results on gold atomic contacts and benzendithiol will be presented.

[1] D. Djukic and J. M. van Ruitenbeek, Nano Lett. 6, 789-793 (2006)
[2] M. Kumar, R. Avriller and J. M. van Ruitenbeek, Phys. Rev. Lett.

108, 146602 (2012)

CPP 21.2 Wed 9:45 H2

Electrical Characterization of Single Molecules via MCBJ — •MATTHIAS WIESER¹, TORSTEN SENDLER¹, SHOU-PENG LIU², SAMUEL WEISBROD², ZHUO TANG², ANDREAS MARX², JANNIC WOLF², ELKE SCHEER², FRANCESCA MORESCO³, GREBING JOCHEN¹, and ARTUR ERBE¹ — ¹Helmholtz-Zentrum Dresden-Rossendorf e.V., D-01328 Dresden — ²Universität Konstanz, D-78457 Konstanz — ³Max Bergmann Center of Biomaterials, D-01069 Dresden

For future molecular electronics applications the detailed knowledge about the electrical transport properties of single molecules is very important. To achieve this goal we are using the mechanical controllable break junction technique in liquid environments in combination with insulating substrates. We characterize the electrical conductance and I-V characteristics of single molecules which consist of three phenyl rings connected by triple carbon bonds with two oxygen sidegroups binding to the central ring. The I-V characteristics are further investigated by creating 2D histograms for hundreds of I-V curves and by fitting a single level model which provides us the metal-molecule

junction coupling constants and the molecular energy level.

CPP 21.3 Wed 10:00 H2

Charge transmission through a molecular junction driven by a time-dependent voltage — ●YAROSLAV ZELINSKY^{1,2}, YORAM SELZER³, and VOLKHARD MAY¹ — ¹Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, D-12489 Berlin, Germany — ²Bogolubov Institute for Theoretical Physics, National Academy of Science of Ukraine, 14-b Metrologichna str., UA-03683, Kiev, Ukraine — ³School of Chemistry, Tel Aviv University, Ramat Aviv, 69978 Tel Aviv, Israel

Time-dependent electron transport through a molecular junction driven by voltage pulses with a duration even in the sub-ps region is investigated theoretically. The transient behavior of the current is analyzed in focusing on the sequential transport regime and in utilizing a density matrix approach. As a quantity detectable in the experiment the averaged dc-current resulting from a sequence of voltage pulses is also calculated. The obtained data are analyzed with respect to their dependence on the voltage pulse shape, the magnitude and asymmetry of the lead-molecule coupling, and the mechanism and strength of intramolecular relaxation. All the findings are confronted with recent computations on transient currents due to optical excitation of the junction [1,2].

[1] L. Wang and V. May, *Phys.Chem.Chem.Phys.* **13**, 8755 (2011)

[2] Y. Zelinsky and V. May, *Nano Lett.* **12**, 446 (2012)).

CPP 21.4 Wed 10:15 H2

Surface Plasmon Enhanced Electroluminescence of a Molecular Junction — ●YUAN ZHANG^{1,2}, YAROSLAV ZHELINSKY¹, and VOLKHARD MAY¹ — ¹Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, D-12489 Berlin, Germany — ²University of Science and Technology Beijing, XueYuan Road 30, 100083 Beijing, P. R. China

There are some first experiments indicating surface plasmon enhanced emission of a molecular junction. We present a coherent theory for this phenomenon, which is based on our previous work on molecule metal nanoparticle complexes [1,2,3,4]. Utilizing a density matrix description our theory accounts for electron transfer in junction, photon emission and energy exchange coupling between the molecule and spherical leads. As a central result, we report on a three order of magnitude enhanced molecular photon emission, which dependence on molecular and junction parameters are also discussed.

[1] Y. Zelinsky, Y. Zhang, and V. May, *J. Phys. Chem. A*, DOI: 10.1021/jp305505c

[2] Y. Zhang, Y. Zelinsky, and V. May, *J. Phys. Chem. C*, accepted

[3] Y. Zhang, Y. Zelinsky, and V. May, *J. Nanophot.*, in press

[4] Y. Zelinsky and V. May, *Nano Lett.* **12**, 446 (2012)

CPP 21.5 Wed 10:30 H2

Dynamics of a nano-scale rotor driven by single-electron tunneling — ALEXANDER CROY² and ●ALEXANDER EISFELD¹ — ¹MPIPKS Dresden — ²Chalmers University of Technology S-412 96 Göteborg, Sweden

We investigate theoretically the dynamics and the charge transport properties of a rod-shaped nano-scale rotor, which is driven by a similar mechanism as the *nanomechanical single-electron transistor (NEM-SET)*. We show that a static electric potential gradient can lead to self-excitation of oscillatory or continuous rotational motion. We identify the relevant parameters of the device and study the dependence of the dynamics on these parameters. We discuss how the dynamics are related to the measured current through the device. Notably, in the oscillatory regime we find a negative differential conductance. The current-voltage characteristics can be used to infer details of the surrounding environment which is responsible for damping.

[1] A. Croy and A. Einfeld, *EPL (Europhys Lett)* **98**, 68004

CPP 21.6 Wed 10:45 H2

First-principles investigation of electron transport through molecular junctions in an STM configuration — ●SHIGERU TSUKAMOTO, VASILE CACIUC, NICOLAE ATODIRESEI, and STEFAN BLÜGEL — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich

Molecular electronics is exciting by the perspective that various types of functionalities are potentially realized only by single molecules with unique electronic structures. A number of interesting experiments on

the transport properties have been performed in an STM configuration, in which a probing tip approaches a molecule on a metal surface.

By means of first-principles methods, we report about a systematic series of calculations on electron transport through molecules in the STM configuration. The molecules to be investigated are a Terephthalic acid molecule and its derivatives, which chemisorb on Cu(110) surfaces.

Electron transmissions are investigated by varying the tip-molecule distance in an STM configuration, as well as by tuning molecular electronic structures. As approaching the tip toward the molecule, some of the transmission peaks originating from unoccupied states move to lower energy due to the hybridization of tip and molecular states. This peak-shift contributes to increasing the electron transmission around the Fermi energy, which is an essential property in molecular devices. This exhibits that in molecular electronics, not only the molecule itself but also the geometrical configuration between a molecule and the electrodes is an important parameter to determine the functionality.

15 min. break

CPP 21.7 Wed 11:15 H2

STM theory for π -conjugated molecules on thin insulating films — ●BENJAMIN SIEGERT, ANDREA DONARINI, SANDRA SOBCHYK, and MILENA GRIFONI — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg

We present a microscopic STM theory, based on the reduced density matrix formalism, which is able to describe transport and topographical properties of interacting π -conjugated molecules on thin insulating films. Simulated current-voltage characteristics and constant height and constant current STM images for a Cu-Phthalocyanine (CuPc) molecule are presented as experimentally relevant examples. We predict negative differential conductance resulting from interference between degenerate many-body states of CuPc [1]. Criteria are given to find and identify the interference blocking scenario in experimental measurements.

[1] A. Donarini, B. Siegert, S. Sobczyk, and M. Grifoni, *PRB* **86**, 155451 (2012).

CPP 21.8 Wed 11:30 H2

Influence of Electronic Properties of Graphene on Current-Voltage Characteristics of Molecule-Graphene Nanojunctions — ●IVAN A. PSHENICHNYUK, PEDRO B. COTO, ANDRÉ ERPENBECK, and MICHAEL THOSS — Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany

Graphene, thanks to its peculiar mechanical and electronic properties, is today considered as a perspective material in future electronics. Its well-known band structure with "zero band-gap" as well as the existence of so-called edge states leads to a non-trivial density of states distribution in graphene-based devices. This causes, in particular, distinctive current-voltage characteristics of molecule-graphene nanojunctions, where a single molecule is connected to two graphene nanosized contacts. We study the transport characteristics of graphene-based nanojunctions using tight-binding models and first-principles DFT calculations combined with the Landauer transport formalism.

CPP 21.9 Wed 11:45 H2

Electron Transport properties of metallic carbon nanotubes with metal contacts — ●ANDREAS ZIENERT¹, JÖRG SCHUSTER², and THOMAS GESSNER^{1,2} — ¹Center for Microtechnologies, Chemnitz University of Technology, Chemnitz, Germany — ²Fraunhofer Institute for Electronic Nano Systems, Chemnitz, Germany

Metallic carbon nanotubes (CNTs) are quasi ballistic one-dimensional conductors capable to carry large current densities. This makes them ideal candidates for applications in future microelectronic devices, partially replacing state-of-the-art copper interconnect lines. The performance of such a system not only depends on intrinsic properties of the CNTs but is also strongly affected by its size and the contact.

We investigate the transport properties of metal-CNT-metal devices theoretically, applying semiempirical (extended Hückel theory) and ab initio (density functional theory) electronic structure methods, combined with a Green's function formalism for ballistic transport at low bias. The study focuses on (6,0) CNTs of different length comparing the metal contacts Al, Cu, Pd, Pt, Ag, Au in a highly symmetric end-to-end configuration.

It turns out that Al forms the most transparent contacts, followed by

Pd, Pt and Cu. The noble metals Au and Ag perform worse. Results are visualized and discussed in terms of the local density of states of the combined metal–nanotube systems and its isolated parts, as well as their contact distances, binding energies, and work functions.

CPP 21.10 Wed 12:00 H2

First principles study of charge and heat transport through π -stacked molecules — ●THOMAS HELLMUTH¹, MARIUS BÜRKLE², FABIAN PAULY³, and GERD SCHÖN¹ — ¹Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — ²Nanosystem Research Institute, National Institute of Advanced Industrial Science and Technology, Japan — ³Theorie der Nanostrukturen, Universität Konstanz, 78457 Konstanz, Germany

We analyze charge and heat transport properties of π -stacked, multi-layered paracyclophane molecules using density functional theory combined with non-equilibrium Green's function techniques. The conductance of that class of molecules was measured in Ref. 1. Beside the elastic conductance we investigate the not yet measured thermopower and inelastic electron tunneling spectra (IETS). The transmission eigenchannels show that the current is mainly carried by the π system of the paracyclophane molecules and by taking into account different contact geometries, we find that this is independent of the binding motif. While the conductance decays exponentially with increasing molecular length, the thermopower increases linearly and may change its sign. Similarly, we analyze how the IETS and the heat transport depend on the molecular length and vibrational modes in the specific junction geometries.

[1] S. T. Schneebeli *et al.* J. Am. Chem. Soc. **133**, 2136 (2011)

CPP 21.11 Wed 12:15 H2

Spin selective transport in chiral systems — ●RAFAEL GUTIERREZ, THOMAS BRUMME, and GIANAURELIO CUNIBERTI — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany

Recent experiments have demonstrated that the transmission of electrons through layers of chiral molecules can be strongly spin-dependent [1,2]. Here, we extend a previous model [3] to discuss the interrelation between the observed effect and the presence of a spin-orbit coupling interaction induced by helical electrostatic fields. Hereby, we

present a minimal model Hamiltonian based on a representation of the Schrödinger equation on a helical pathway and discuss the influence of several parameters on the spin polarization. Complementary to it, full 3D wave packet propagation is discussed in the presence of spin-orbit coupling. Our results suggest that a spin polarization can be induced as a result of the symmetry of the system. However, it appears that a full 3D description of the problem may be necessary.

[1] B. Goehler, V. Hamelbeck, T. Z. Markus, M. Kettner, G. F. Hanne, Z. Vager, R. Naaman, H. Zacharias, Science **331**, 894 (2011)

[2] Z. Xie, T. Z. Markus, S. R. Cohen, Z. Vager, R. Gutierrez, R. Naaman, Nano Letters **11**, 4652 (2011)

[3] R. Gutierrez, E. Diaz, R. Naaman, G. Cuniberti, Phys. Rev. B **85**, 081404(R) (2012)

CPP 21.12 Wed 12:30 H2

Full ab initio description of strong electronic correlations in molecular devices — ●DAVID JACOB — Max-Planck-Institut für Mikrostrukturphysik, Halle

In order to obtain a *full* first-principles description of the correlated electronic structure and transport properties of nanoscopic devices we combine the so-called Coulomb-Hole-Screened-Exchange (COHSEX) approximation with more sophisticated many-body techniques such as the Dynamical Mean-Field Theory (DMFT). While the former yields an effective mean-field description of the weakly correlated conduction electrons, the latter describes the dynamic correlations of the strongly interacting electrons in the $3d$ - or $4f$ -shells of transition metal atoms. The combination of DMFT with COHSEX instead of Density Functional Theory (DFT) improves upon our recently developed "Molecular DMFT" approach [1,2] in two important aspects: First, the COHSEX yields the effective Coulomb interaction U for the strongly interacting electrons. Second, unlike in DFT+DMFT calculations the double-counting correction for COHSEX+DMFT is exactly known and straight-forward to calculate. With this approach it is now possible to actually predict e.g. the occurrence of the Kondo effect in magnetic atoms and molecules on metal surfaces and attached to metallic leads, and to investigate the complex nature of the Kondo effect in these systems.

[1] D. Jacob *et al.*, PRL **103**, 016803 (2009); PRB **82**, 195115 (2010)

[2] M. Karolak *et al.*, PRL **107**, 146604 (2011)

CPP 22: Focus: Wetting on smooth and rough surfaces: From spreading to superhydrophobicity I

Wetting determines the morphology and dynamics of a liquid on a surface. In particular for rough, structured, or deformable surfaces the dynamic contact angles are poorly understood. Progress in experimental and numerical techniques permit time resolved three-dimensional investigations of wetting, providing new insight into the interplay between the contact angle, hysteresis, and pinning.

Organizers: Hans-Jürgen Butt (Mainz), Stephan Herminghaus (Göttingen), Doris Vollmer (Mainz)

Time: Wednesday 9:30–13:00

Location: H34

Invited Talk

CPP 22.1 Wed 9:30 H34

Liquid drops on soft solids — ●JACCO SNOEIJER — University of Twente, The Netherlands

The wetting of a liquid on a solid usually assumes the substrate to be perfectly rigid. However, this is no longer appropriate when the substrate is very soft: capillary forces can induce substantial elastic deformations, as has been demonstrated e.g. for drops on elastomers. In this talk we discuss the fundamentals of elasto-capillary interactions. Theory, simulations and experiments reveal the surprising nature of capillary forces, which turn out to be different from anything proposed in the literature. We also discuss how the law for the contact angle (Young's law) is modified for soft substrates.

CPP 22.2 Wed 10:00 H34

How soft viscoelastic surfaces control the time scales of drop spreading — LONGQUAN CHEN¹, ●ELMAR BONACCURSO¹, and MARTIN SHANAHAN² — ¹Center of Smart Interfaces, Technische Universität Darmstadt, Petersenstr. 17, 64287 Darmstadt, Germany — ²Univ. Bordeaux, I2M, UMR 5295, F-33400 Talence, France

It is known that liquid droplets spreading on a soft, viscoelastic substrate can be slowed down considerably by the formation of a wetting

ridge, or protrusion of the substrate near the triple phase contact line (TPCL) due to capillary forces. Viscoelastic dissipation in the substrate can prevail over viscous dissipation in the liquid and dominate the spreading process. In this contribution we show how the internal time scales of the viscoelastic solid interact with a spreading droplet.

After contact of a droplet and a viscoelastic substrate a short, rapid spreading stage occurs. The necessary balance determining speed of motion of the TPCL is initially between capillary and inertial forces. As spreading proceeds, inertia lessens while the lower spreading speed allows for viscoelastic effects to emerge. We study the transition between inertial and viscoelastic regime by high-speed video microscopy and propose a simple model for relating the transition time with properties of the liquid and the viscoelastic substrate.

CPP 22.3 Wed 10:15 H34

The wetting properties of graphene in the light of molecular dynamics simulations — ●FRÉDÉRIC LEROY, FERESHTE TAHERIAN-TABASI, VALENTINA MARCON, and NICO VAN DER VEGT — Center of Smart Interfaces, TU Darmstadt, Darmstadt, Germany

It has recently been shown that monolayer graphene may serve as a protective coating for metals and nonpolar solid substrates while preserving the wetting properties of these surfaces with respect to water.

The question arises as to whether such coating would preserve the wetting properties of all nonpolar surfaces.

To answer this question, the contact angle of water droplets on suspended isolated graphene must be known. Experimental work suggests that graphene may yield a value of the contact angle as high as 127° , whereas other studies suggest a weak enhancement in comparison with the value of 95° on graphite.

We have developed an argumentation supported by molecular dynamics simulations to show that a value of the contact angle of water on graphene cannot exceed 100° . In agreement with recent experimental work, it is thus anticipated that graphene coating is not transparent to the wetting properties of nonpolar substrates which yield contact angles larger than 100° .

Furthermore, our study leads to the conclusion that the work of adhesion of water on graphene includes a non-negligible entropy contribution. Based on the theory of solvation, we introduce the idea that this entropy contribution is related to the fluctuations in the water-substrate interaction energy.

CPP 22.4 Wed 10:30 H34

History-dependent dynamic receding contact angles of aqueous surfactant solution slugs flowing through polymeric capillaries — MANOS ANYFANTAKIS, DANIELA FELL, HANS-JÜRGEN BUTT, and GÜNTER K. AUERNHAMMER — Max Planck Institute for Polymer Research, Mainz, D-55128, Germany

The time-dependent dewetting behavior of surfactant solution slugs which are forced to move in fluorinated ethylene propylene (FEP) micro-tubes was experimentally investigated. The dynamic receding contact angle at a given wetting velocity, measured by high-speed imaging of the receding menisci, was found to decrease as the solid-liquid contact time increased. Long-time kinetics of several hundred s led to a final state displaying a 0o dynamic receding contact angle. The receding contact angle kinetics was found to strongly depend on the slug velocity. Higher speeds led to a faster decrease in the receding contact angles. Qualitatively similar results were obtained for anionic (sodium dodecyl sulfate) and cationic (hexadecyltrimethylammonium bromide) aqueous surfactant solutions at concentrations below and equal to the corresponding critical micellar concentration. Employing a different hydrophobic surface (polycarbonate micro-tubes) led to an analogous dewetting behavior, presumably indicating a generic effect for hydrophobic solid surfaces. This history effect was absent in simple liquids (2-propanol, water), where the dynamic receding contact angle does not depend on the contact time.

M. Anyfantakis et al., Chem. Lett. 2012, 41, 1232

CPP 22.5 Wed 10:45 H34

Mixed Wettability on the Mesoscopic scale: Effect of wetting correlation length in porous media — JULIE MURISON¹, BENOIT SEMIN², JEAN-CHRISTOPHE BARET¹, STEPHAN HERMINGHAUS¹, MATTHIAS SCHRÖTER¹, and MARTIN BRINKMANN¹ — ¹Max Planck Institute of Dynamics and Self Organisation, Göttingen, Germany — ²Laboratoire de Physique Statistique, ENS, Paris, France

In order to better understand the behavior of immiscible two phase flow through mixed wetting porous media, we have designed a series of experiments to test the effect of isolated and controlled microscopic heterogeneities (sub-grain) on a larger sample scale (20 mm). Here we present the effect of wetting correlation length on the sub-pore to multi-pore (aprox 1mm) scale. Initial results indicate that sample composition alone cannot adequately describe the fluids behavior, but rather the size of the heterogeneity creates different wetting environments. In particular sub-pore heterogeneity causes large hysteresis in fluid displacement profiles. Recently we combine gravimetric measurements of fluid displacement with X-ray microtomography to characterise and quantify effective trapping environments for droplets within the porous media.

CPP 22.6 Wed 11:00 H34

Dewetting of mixtures as described by a gradient dynamics model — UWE THIELE, DESISLAVA TODOROVA, and HENDER LOPEZ — Department of Mathematical Sciences, Loughborough University, Loughborough, Leicestershire, LE11 3TU, UK

We show that the dynamics of free surface films of mixtures (polymer blends, nanoparticle suspensions) may be described by a hydrodynamic long-wave model that is written thermodynamically inspired gradient dynamics form based on an underlying free energy functional (accounting for wettability and capillarity). For an ideal mixture whose components do not differ in their wettability, the *classical* hydrodynamic

model used, e.g., in Refs. [1,2] is recovered. The gradient dynamics form allows us to extend the model to incorporate (i) solute-dependent wettability, and (ii) solute-solvent decomposition [3]. We illustrate extension (i) by an investigation of the dewetting of a film of a mixture and show that a film may become unstable through the coupling of film height and concentration fluctuations. The resulting nonlinear dynamic behaviour and equilibrium states are discussed [4]. The outlook discusses how the idea also applies to surfactant-covered films [5]. We acknowledge support by the EU (PITN-GA-2008-214919).

[1] M. Warner, R. Craster and O. Matar. J. Colloid Interface Sci. 267, 92 (2003). [2] L. Frastia, A.J. Archer, U. Thiele, Phys. Rev. Lett. 106, 077801 (2011); Soft Matter 8, 11363 (2012). [3] U. Thiele, Eur. Phys. J. Special Topics, 197, 213-220 (2011). [4] D. Todorova, H. Lopez and U. Thiele, in prep. [5] U. Thiele, A.J. Archer and M. Plapp, Phys. Fluids 24, 102107 (2012).

15 min. break

Invited Talk

CPP 22.7 Wed 11:30 H34

Wetting transitions in polymer decorated nanostructured surfaces — JÜRGEN RÜHE — Institut für Mikrosystemtechnik, Universität Freiburg, 79110 Freiburg

We describe the generation of well defined micro- and nanostructured surfaces with surface-attached polymer monolayers. To this high aspect ratio micro- and nanostructured surfaces are generated in silicon through lithography, the Bosch process or DRIE process. In the first case well defined post structures, in the latter silicon nanogras structures are obtained. The silicon structures are coated with self-assembled monolayers containing benzophenone groups. These monolayers are used for a photoinduced attachment of polymer monolayer to these surfaces. We study the wetting properties of such surfaces as a function of the surface energy of the polymer involved. Superwetting, Wenzel-type of wetting and superhydrophobic properties can be observed. In some cases roll-off angles well below $<1^\circ$ are observed. It is found that such surfaces show very distinct wetting transitions, where even minor changes in the surface energy of the coating cause huge changes in the contact angle.

CPP 22.8 Wed 12:00 H34

Dynamics of water droplets on nanostructured hydrophobic surfaces with step gradients — TOBIAS NECKERNUSS, STEFAN WIEDEMANN, ALFRED PLETTL, and PAUL ZIEMANN — Institute of Solid State Physics, University of Ulm

Droplets on a surface exhibiting different contact angles (CA) along their three-phase-contact-line experience a net force due to uncompensated Young forces. These forces play a major role in the dynamics of both, CA hysteresis and gradient-induced movement. A simple analytical model is developed based on these uncompensated Young components combined with geometrical constraints when a droplet laterally crosses a wettability step. Such steps are prepared with a micellar technique in combination with a hydrophobic Teflon-like coating leading to arrays of nanopillars (typical height: 100 nm, diameter: up to 40 nm). As a result, CAs of about 165° and 150° are observed for advancing and receding droplets, respectively. By varying parameters like pillar density and diameter, the forces acting on a moving droplet can be adjusted. The dynamics of moving droplets are investigated with a modified commercial CA measurement setup. To move a droplet towards the wettability step, the substrate can be tilted, allowing control of its shape and velocity in the vicinity of the step. Comparison of experimental data to the model prediction shows remarkable agreement.

CPP 22.9 Wed 12:15 H34

Dynamic Measurement of the Force Required for Moving a Liquid Drop on a Solid Surface — DOMINIK PILAT, PERIKLIS PAPADOPOULOS, DAVID SCHÄFFEL, DORIS VOLLMER, RÜDIGER BERGER, and HANS-JÜRGEN BUTT — Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany

A novel setup for direct measurement of the force needed to move a drop on a solid surface was developed. The forces were measured by means of a vertical deflectable capillary stuck in the drop. The drop adhesion force instrument (DAFI) allowed us to investigate the dynamic lateral adhesion force of water drops of 0.1 to 2 μL volume at defined velocities. On flat PDMS surfaces, the dynamic lateral adhesion force increases linearly with the diameter of the contact area of the solid liquid interface and linearly with the sliding velocity. We further investigated a 3D superhydrophobic pillar array. The depinning of the

receding part of the rim of the drop occurred almost simultaneously for four to five pillars, giving rise to peaks in the lateral adhesion force. The spatial resolution of the lateral adhesion force, which is possible with the DAFI, is not only interesting for scientific applications, but also for industrial applications like quality control of surfaces made in large scale processes.

CPP 22.10 Wed 12:30 H34

Exploring the high-pressure wetting resistance of springtail skin by in situ plastron collapse tests and numerical simulations — ●RENÉ HENSEL¹, RALF HELBIG¹, JULIA NICKERL¹, SEBASTIAN ALAND², HANS-GEORG BRAUN¹, AXEL VOIGT², CHRISTOPH NEINHUIS^{3,4}, and CARSTEN WERNER^{1,4} — ¹Max Bergmann Center of Biomaterials, Leibniz Institute of Polymer Research Dresden, Germany — ²Institute of Scientific Computing, TU Dresden, Germany — ³Institute of Botany, TU Dresden, Germany — ⁴B CUBE Innovation Center for Molecular Bioengineering, TU Dresden, Germany

Springtails (Collembola), wingless arthropods are adapted to cutaneous respiration in temporarily rain-flooded habitats due to a non-wetting skin surface. They immediately form a plastron protecting them against suffocation upon immersion into water and even low-surface-tension liquids. Herein, we present the design principles for pressure resistance of such plastrons against collapse. Therefore, the skin morphology of springtails was studied by transmission electron microscopy. The micrographs reveal cavity side-wall profiles with characteristic overhangs. These were fitted by polynomials to allow access for analytical calculations of the breakthrough pressure, i.e., the barrier against plastron collapse. The actual dynamics of an enforced wetting transition from heterogeneous to homogeneous wetting state were performed by in situ plastron collapse tests and numerical simulations based on a diffuse interface approach for two phase flow. Furthermore, model

profiles with well-defined geometries were used to develop a general design principle for the most robust surface structures.

CPP 22.11 Wed 12:45 H34

Design of the self-repairable materials using colloidal particles — ●NIKOLAY PURETSKIY^{1,2}, GEORGI STOYCHEV^{1,2}, ALLA SYNYTSKA¹, and LEONID IONOV¹ — ¹Leibniz-IPF Dresden, 01069 Dresden, Germany — ²TU Dresden, 01062 Dresden, Germany

We suggest an approach for the design of materials with self-repairable switchable and hydrophobic properties. The approach is based on use of colloidal particles located on a surface of hydrophobic oil. Due to surface forces, the colloidal particles segregate at the wax surface after melting and change its wetting properties. Since the degree of particle immersion in the wax depends on the environment (hydrophilic or hydrophobic), the roughness, as well as the wetting properties of the particle-wax composite surface, can be switched. The obtained morphology can be "frozen" by cooling down below oil melting point [1]. Notably, since the colloidal particles are homogeneously distributed in the wax bulk, removal of the topmost particle-wax layer does not result in disappear of switchable properties. After remelting the particles segregate again at newly formed surface and switchable properties are recovered. The similar approach is used for the design of materials with self-repairable ultrahydrophobic properties. The materials are based on perfluorinated decane with incorporated colloidal particles. Due to the highly pronounced tendency of this perfluorinated decane to crystallize, the formation of blends with rough fractal surfaces was observed [2]. [1] N. Pureskiy, G. Stoychev, M. Stamm and L. Ionov; ACS Applied Materials and Interfaces, 2010, 2, 2944-2948 [2] N. Pureskiy, G. Stoychev, A. Synytska and L. Ionov; Langmuir, 2012, 28, 3679-3682

CPP 23: Polymer Dynamics

Time: Wednesday 9:30–13:00

Location: H39

Invited Talk

CPP 23.1 Wed 9:30 H39

Polymers, rings and pores: A neutron scattering study — ●ANDREAS WISCHNEWSKI — Jülich Centre for Neutron Science JCNS-1 and Institut for Complex Systems ICS-1, Forschungszentrum Jülich, Germany

Polymers are one of the most important and fascinating soft matter materials both from the fundamental point of view as well as with respect to their wide range of applications. Industrial processing, design, fabrication and application depends to a large extend on the understanding of the rheological properties on a microscopic level. Neutron scattering is a powerful tool to access the microscopic characteristics of polymeric systems and has already significantly contributed to the understanding of the static and dynamic properties of polymers with different architectures and in different, complex environments. Recently, ring polymers have attracted ample interest both from simulation experts and experimentalists. The absence of chain ends, which determine the dynamics of linear chains and in particular branched polymers, allows to examine fundamental aspects of polymer theory. Neutron spin echo spectroscopy reveals significant differences in ring dynamics compared to the linear counterpart. In particular rings cannot build up easily the tube confinement as known from long linear chains. In contrast to that, polymers in nano-pores are subject to a stronger topological confinement as compared to the bulk system if a surface-polymer interaction is present. Neutron scattering studies combined with complementary techniques are presented.

CPP 23.2 Wed 10:00 H39

The collapse transition of poly(2-oxazoline) gradient copolymers - a multistep process — SEBASTIAN JAKSCH¹, KONSTANTINOS KYRIAKOS¹, JIANQI ZHANG¹, ISABELLE GRILLO², ANITA SCHULZ³, RAINER JORDAN³, and ●CHRISTINE M. PAPADAKIS¹ — ¹TU München, Physik-Department, Physik weicher Materie, Garching — ²Institut Laue-Langevin, Grenoble — ³TU Dresden, Department Chemie, Professur für Makromolekulare Chemie

Thermoresponsive poly(*iso*-propyl-2-oxazoline) (PiPrOx) polymers in aqueous solution exhibit a strong change in solubility and chain conformation when heated above their cloud point (CP). The CP decreases strongly upon insertion of few hydrophobic monomers.

We investigated poly(*iso*-propyl-2-oxazoline)-*grad*-(*n*-nonyl-2-oxazoline) (P[*i*PrOxNOx]_{*grad*}) gradient copolymers with a varying fraction of NOX moieties. In temperature-resolved SANS experiments, we have found a two-step collapse and aggregation behavior of the gradient copolymers at the cloud point which is not present in the homopolymer [1]. Time-resolved SANS allowed us to monitor the structural evolution of the aggregates when rapidly heating the solutions from below the CP to different temperatures above. We found that, the higher the target temperature, the more pronounced is the collapse. Moreover, the aggregates present in the intermediate regime are stable and do not transform into those found at higher target temperatures.

[1] S. Salzinger, S. Jaksch, C.M. Papadakis et al., *Colloid Polym. Sci.* **290**, 385 (2012).

CPP 23.3 Wed 10:15 H39

Local, global and collective dynamics in a short polymer system. — ●HUMPHREY MORHENN^{1,2}, SEBASTIAN BUSCH³, and TOBIAS UNRUH² — ¹Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II) and Lehrstuhl für Funktionale Materialien, Technische Universität München, Germany — ²Lehrstuhl für Kristallographie und Strukturphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — ³Department of Biochemistry, University of Oxford, United Kingdom

The *n*-alkane C₁₀₀H₂₀₂ is an oligomer on the edge of being a polymer. Although its chains are shorter than the entanglement length and long enough to show Gaussian chain statistics, the Rouse model fails to predict the chain dynamics. Detailed quasielastic neutron scattering experiments and extensive molecular dynamics simulations were performed, providing complementary pictures on the molecular motions. Three distinct relaxation processes on the pico- to nanosecond time regime were separated, eventually leading to molecular self-diffusion. Two relaxations were found to correspond to local torsional and global rotational motions of single molecules, whereas a third, intermediate relaxation can be explained by intermolecular collective motions. Taking these contributions into account a physical model describing molecular self-diffusion is being developed.

CPP 23.4 Wed 10:30 H39

Selective Solid-State NMR Investigations of Polymer Dynamics — UTE BÖHME, ANASTASIA VYALIKH, and •ULRICH SCHELER — Leibniz-Institut für Polymerforschung Dresden e.V.

NMR relaxation provides information on the molecular dynamics over a wide range of correlation times. To achieve spectral resolution in solid polymers high-resolution solid-state NMR based on CRAMPS (combined multipulse and rotation spectroscopy) has been applied. The spectral resolution permits to resolve different components in copolymers and mixtures in proton NMR spectra. The sensitivity in the proton spectra will permit the study of thin films as well. Selective swelling of single components which is accompanied by enhanced segmental dynamics has been observed in both spin-spin-relaxation (T2) and spin-lattice relaxation in the rotating frame (T1rho). Spectral resolution permits the identification of the components and assignments of their local mobility.

CPP 23.5 Wed 10:45 H39

Studies of entangled polymer dynamics by NMR: validity of tube model variants and nanoparticle effects — •FILIPE FURTADO¹, JOSHUA DAMRON¹, MARIE-LUISE TRUTSCHER¹, MANSI AGARWAL², CHARLES ZUKOSKI², and KAY SAALWÄCHTER¹ — ¹Institut f. Physik-NMR, Martin-Luther-Univ. Halle, Deutschland — ²University of Illinois at Urbana-Champaign, USA

The validity of fixed-tube model remains a matter of intense debate. Ongoing discussions include the dynamics of the tube itself and of contour-length fluctuations (CLF) and constrained release (CR) effects. Suitable NMR experiments [1] were used to investigate CR effects by probing the dynamics of diluted protonated polybutadiene (PB) chains in matrices of deuterated (NMR-invisible) high molecular weight PB chains. Such dilution experiments have been reported to be subject to a bias due to interchain correlations in NMR T1 relaxation experiments [2], but these effects have been shown to not significantly affect our experiments. CLF was investigated on deuterated pseudotriblock copolymers (2H-1H-2H). Furthermore, we hereby present the first NMR experiments clearly confirming the recently predicted nanoparticle effect on chain disentanglement [3] on a molecular scale by monitoring the influence of polyhedral oligomeric silsesquioxanes (POSS) on the disentanglement time of polyethyleneoxide melts.

[1] F. V. Chávez et al., Phys. Rev. Lett., 2010, 104, 198305

[2] A. Herrmann et al., Macromolecules, 2012, 45, 6516

[3] Y. Li et al., Phys. Rev. Lett., 2012, 20121, 09, 118001

CPP 23.6 Wed 11:00 H39

Deformation Dynamics of Thin Stretched Polymer Films — •STEFAN KRAUSE, MARTIN NEUMANN, MELANIE BIBRACH, ROBERT MAGERLE, and CHRISTIAN VON BORCZYKOWSKI — Fakultät für Naturwissenschaften, TU Chemnitz, D-09107 Chemnitz

The fluorescence of polymer embedded reporter molecules reacts very sensitive on environmental changes such as mechanical stress. Especially polarization effects of these fluorophores allow for the spatial and temporal observation of the deformation within drawn polymer films while the utilization of ultra sensitive force sensors enables to measure the global mechanical deformation behaviour of the polymer film. We report on fluorescence (single molecule) microscopy, atomic force and mechanical force investigations of thin films of viscoelastic polymethylacrylate (PMA). The films are stretched using a micro tensile testing setup. Simultaneously, peryleneimide dyes functionalized with different side chains were embedded in the film and report via their molecular dynamics changes within their local environment.

15 min. break

CPP 23.7 Wed 11:30 H39

Dynamics of Regular Hyperbranched Polymers — •FLORIAN FÜRSTENBERG, MAXIM DOLGUSHEV, and ALEXANDER BLUMEN — Theoretische Polymerphysik, Universität Freiburg, Hermann-Herder-Str.3, D-79104 Freiburg, Deutschland

Theoretical investigations of hyperbranched polymers are enjoying growing attention. Up to now, analytic work focused on regular fully-flexible hyperbranched polymers such as dendritic structures. Here we investigate the dynamics of semiflexible dendrimers of arbitrary functionality f and generation g . We focus on the solution of the corresponding Langevin equations which can be formulated in an analytic form^[1]. Moreover, we show that the corresponding diagonalization problem can be drastically simplified by using a complete set of eigenmodes, which is similar to the set for fully-flexible den-

drimers known from the literature^[4,5]. Another advantage of our diagonalization scheme is that it provides automatically the eigenvalues' degeneracies^[4]. The presented scheme for dendrimers paves the way for theoretical investigations of more complex polymeric architectures^[5].

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

[2] C. Cai and Z.Y. Chen, Macromolecules **30**, 5104 (1997).

[3] A. A. Gurtovenko, D.A. Markelov, Y.Y. Gotlib, and A. Blumen, J. Chem. Phys. **119**, 7579 (2003).

[4] F. Fürstenberg, M. Dolgushev, and A. Blumen, J. Chem. Phys. **136**, 154904 (2012).

[5] F. Fürstenberg, M. Dolgushev, and A. Blumen, submitted.

CPP 23.8 Wed 11:45 H39

Unwinding polymer globules under stretching force: A Monte Carlo study — •CHRISTOPH JENTZSCH^{1,2}, MARCO WERNER^{1,2}, and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden, Germany — ²Technische Universität Dresden, Germany

We investigate linear polymer chains under poor- and non-solvent conditions using the bond fluctuation model with explicit solvent. By implementing many-body effects implicitly, this model allows for free diffusion of polymer globules under non-solvent conditions on the same time scale as in good solvent while keeping the computational effort low as compared to off-lattice calculations. We analyze static and dynamic properties of polymer globules in poor solvent. We further calculate the force acting on chain ends, when they are fixed at a given distance. Our results for the force-extension curve are qualitatively in good agreement with recent experiments and with numerical results using a self-consistent field approach. For distances slightly larger than the globule diameter, we observe a tadpole regime where one stretched part of the chain is in equilibrium with a single residual globule. The force necessary to form a stable tadpole conformation as function of solvent quality can be understood using scaling arguments based on the thermal blob size. For increasing distances, we observe a decay of the tadpole into smaller globules and stretched chain parts. Here, the stretching force shows a local minimum and a quantitative explanation for the observed shape of the force-extension curve remains a challenge. For larger distances a cross-over to a strongly stretched chain behavior is found.

CPP 23.9 Wed 12:00 H39

Translocation of macromolecules with different architectures through polymer brush covered microchannels — •IRINA NERATOVA¹, TORSTEN KREER¹, and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Straße 6, D-01069 Dresden, Germany — ²Technische Universität Dresden, Institut für Theoretische Physik, Zellescher Weg 17, D-01069, Dresden, Germany

Polymer brush covered channels have attracted a lot of attention in recent years for both engineering and biomedical applications. They play an important role in the design of novel microfluidic devices, the control of targeted drug delivery, stabilization of colloids, and lubrication. Although the equilibrium properties of polymer brushes are well understood, many non-equilibrium phenomena have not been studied to date. One example is the translocation of macromolecules through a brush covered microchannel.

In this study, Molecular Dynamics simulations are employed to investigate the influence of the architecture of macromolecules on their ability to pass through a brush covered channel. The properties of linear and star polymers embedded in the microchannel are studied in thermodynamic equilibrium and within Poiseuille flows of various strengths. It is shown that, in equilibrium, a linear macromolecule diffuses faster than a polymer star of the same molecular weight. On the other hand, a pressure gradient may be regarded as a driving force for faster motion of the star polymer.

CPP 23.10 Wed 12:15 H39

A Simulation Study of the Lithium Transport Mechanism in Ternary Polymer Electrolytes – The Critical Role of the Segmental Mobility — •DIDDO DIDDENS and ANDREAS HEUER — Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster

Polymer electrolytes – typically consisting of PEO and a lithium salt such as LiTFSI – are promising candidates for light-weighted but powerful energy storages. However, at ambient temperatures, the con-

ductivity of most polymer electrolytes is still too low for an efficient technological use. Among several other remedies, the incorporation of an ionic liquid (IL) seems to be a fruitful improvement of these materials. Here, it was observed that depending on the ratio of PEO ether oxygens to lithium ions, the lithium diffusion coefficient significantly increases with the IL concentration or, alternatively, is roughly constant [Passerini *et al.*, *Electrochim. Acta*, 2012]. In order to unravel the microscopic scenario giving rise to these observations, we use MD simulations in combination with a Rouse-based analytical transport model, which has originally been devised for classical polymer electrolytes. It turns out that the mobility of the PEO segments plays a decisive role for the precise value of the macroscopic lithium diffusion constant due to the cooperative motion of the lithium ions with the polymer segments. For the latter, two opposing effects are present in the ternary systems: the slowing-down due to the coordinating lithium ions and the plasticizing effect of the IL. Thus, for the design of novel battery materials, one should ensure that the latter effect dominates.

CPP 23.11 Wed 12:30 H39

Multi-scale Modelling of Phase Inversion Membranes — ●RICHARD J BROADBENT, JAMES S SPENCER, ANDREW G LIVINGSTON, ARASH A MOSTOFI, and ADRIAN P SUTTON — Imperial College London, United Kingdom

It is expected that by 2025 two-thirds of the world's population will live in countries with water supply problems[1]. Separation processes account for 40-70% of capital and operating costs in industry[2]. Membrane technology is expected to be key to addressing both these issues. Organic solvent nano-filtration membranes are widely used by industry.

Understanding and predicting the performance of nano-filtration membranes remains unsolved and is an area in which theory and simulation is yet to have a major impact. One of the challenges for the development of accurate and predictive models of the structure of polymer membranes is that they must span multiple length- and time-scales: the membranes are manufactured over a period of seconds from chemicals which diffuse on a picosecond time scale; the

pores within the membranes are often less than a nanometer in size, while the polymers they are made from are often almost a micrometer long. By combining Density Functional Theory, Molecular Dynamics and Monte Carlo methods it is possible to capture all these key scales and advance our understanding of this important technology.

[1] <http://www.un.org/ecosocdev/geninfo/sustdev/waterrep.htm>

[2] Jimmy L. Humphrey and George E. Keller II. Separation Process Technology. New York, McGraw-Hill, 1997.

CPP 23.12 Wed 12:45 H39

Interplay of morphology and rheology during foaming of block copolymers of polystyrene and poly(methyl methacrylate) — GOLDA LOUIS CHAKKALAKAL¹, ●ULRICH A. HANDGE¹, ULLA VAINIO², and VOLKER ABETZ¹ — ¹Institute of Polymer Research, Helmholtz-Zentrum Geesthacht, Max-Planck-Straße 1, 21502 Geesthacht, Germany — ²Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg

Porous and cellular polymers are technologically used in a variety of applications, e.g. in lightweight applications or for acoustic and thermal insulation. Furthermore, porous polymers with an open-cell structure can be used as membranes for microfiltration purposes. If a block copolymer is chosen for preparation of a porous or cellular polymer, then the phenomenon of microphase-separation yields an additional degree of freedom to prepare nanostructured materials. In this study, we systematically investigate the influence of morphological and rheological properties on the preparation of foams of polystyrene (PS)-*b*-poly(methyl methacrylate) block copolymers. The foams were prepared using the technique of batch foaming with carbon dioxide as blowing agent. The analysis of rheological data reveals that molecular weight and morphology strongly influence the complex modulus and the creep compliance. The solution of carbon dioxide in PS-*b*-PMMA block copolymers leads to a reduction of the glass transition temperature of the PS and the PMMA phase. Generally, foaming of PS-*b*-PMMA block copolymers with a cylindrical morphology leads to foams with a lower density than the foams with a lamellar morphology.

CPP 24: Organic Semiconductors

Time: Wednesday 9:30–13:00

Location: H40

Invited Talk

CPP 24.1 Wed 9:30 H40

Factors determining the contact resistance in organic thin-film transistors — MANFRED GRUBER¹, ●EGBERT ZOJER², FERDINAND SCHÜRRER¹, and KARIN ZOJER¹ — ¹Institute of Theoretical and Computational Physics, Graz University of Technology, A-8010 Graz, Austria — ²Institute of Solid State Physics, Graz University of Technology, A-8010 Graz, Austria

The contact resistance is known to severely hamper the performance of organic thin-film transistors. This is particular true when dealing with large injection barriers, high mobility organic semiconductors, or short channel lengths. A common assumption is that the primary quantity determining the value of the contact resistance is the injection barrier at the source electrode. Using drift-diffusion based simulations we show that in sharp contrast to this assumption also the actual device geometry (top- vs. bottom contact), the mobility of the used active material as well as the operation condition of the device can change the contact resistance by several orders of magnitude.[1] The final value of the contact resistance arises from a subtle interplay of all these factors as it is crucially determined by local fields and carrier densities. We also find that the dominant mode of injection (thermionic vs. tunneling) is strongly affected by the above parameters and that (in analogy with the findings of Brondijk *et al.* [2]) the inclusion of barrier shaping fields, mirror charge effects and recombination at the electrode surfaces [3] is essential to obtain qualitatively meaningful results. [1] Adv. Funct. Mater., *prov. accepted*, [2] Org. El. 13, 1526 (2012); [3] Org. El. 13, 1887 (2012)

CPP 24.2 Wed 10:00 H40

Stochastic modeling of molecular charge transport networks — ●OLE STENZEL¹, BJOERN BAUMEIER², CARL POELKING², DENIS ANDRIENKO², and VOLKER SCHMIDT¹ — ¹Ulm University, Ulm, Germany — ²Max Planck Institute for Polymer Research, Mainz, Germany

Theory and simulations have substantially contributed to our understanding of charge and energy transfer processes in amorphous organic semiconductors.[1] In this talk, we present a stochastic network model for charge transport simulations in amorphous organic semiconductors, which generalizes the correlated Gaussian disorder model to more realistic (off-grid) morphologies, where the information on positional disorder (and other properties) are gained by microscopic simulations.[2] The network model is based on tools from stochastic geometry. It includes an iterative dominance-competition model for positioning hopping sites in space, distance-dependent distributions for the vertex connectivity and electronic coupling elements, and a moving-average procedure for spatially correlated site energies. The field dependence of the hole mobility of the amorphous organic semiconductor, tris-(8-hydroxyquinoline)aluminum, which was calculated using the stochastic network model, showed good quantitative agreement with the prediction based on a microscopic approach. The stochastic model can be used to simulate large system sizes in realistic device geometries.

[1] V. Rühle *et al.*, J. Chem. Theory Comput., 2011, 7 (10), 3335-3345

[2] B. Baumeier *et al.*, Phys. Rev. B, 2012, 86, 184202

CPP 24.3 Wed 10:15 H40

The Impact of energetic disorder on the charge transport in organic molecular crystals — ●SEBASTIAN RADKE, RAFAEL GUTIERREZ, and GIANAURELIO CUNIBERTI — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany

In a theoretical study combining molecular dynamics simulations, quantum-chemical calculations, and Marcus theory-based charge migration simulations, we investigate the electronic structure and the charge transport of three members of a promising class of organic near-infrared absorber materials: aza-BODIPYs, which are partially already successfully used as the donor material in organic solar cells.[1] The local character of the frontier molecular orbitals and their coupling to

the intramolecular dynamics significantly influence the size of the total charge carrier mobility and determine whether a material has a higher electron or hole conductance. These effects depend also on the molecular packing and correspondingly on steric effects causing differences in the ratio between the electron and the hole mobility of highly ordered materials. Interestingly, the fluctuations of the transfer integrals can influence both the total value of the charge carrier mobility as well as its anisotropy. This demonstrates that both local and non-local energetic disorder effects have to be considered to formulate design rules for the class of aza-BODIPY derivatives to help to further improve the efficiency of organic solar cells.

[1] T. Mueller et al. *Solar Energy Materials & Solar Cells* 99, 176-181 (2012).

CPP 24.4 Wed 10:30 H40

A comprehensive picture of p-doping P3HT with the molecular acceptor F₄TCNQ — ●PATRICK PINGEL and DIETER NEHER — Institute of Physics and Astronomy, University of Potsdam, D-14476 Potsdam

Molecularly doped semiconducting polymers can exhibit exceptionally high electrical conductivity, making them suitable for use in solution-processed organic circuitries. It has, however, been shown that the density of the created free charges is well below the density of applied dopant molecules, which has been attributed to aggregation of the dopants and/or insufficient charge carrier dissociation. We used optical absorption spectroscopy, surface potential and conductivity measurements to unravel the mechanism leading to reduced doping efficiency in blends of poly(3-hexylthiophene), P3HT, doped with tetrafluorotetracyanoquinodimethane, F₄TCNQ. Within the broad range of doping ratios investigated, we find that almost every F₄TCNQ dopant undergoes full charge transfer with a P3HT donor site. The majority of these charge pairs remains, however, strongly bound and only ca. 5% of the doping-induced holes on P3HT are mobile and contribute to electrical conduction. The conductivity turns from a sublinear increase (i.e., a decrease of mobility) at low-to-moderate doping ratios towards a superlinear increase at high doping ratios. This dependency is quantitatively reproduced applying a numerical mobility model of Arkhipov et al. [*Phys. Rev. B* 72, 235202 (2005)], which considers the broadening of the energetic landscape for charge transport upon doping by the Coulomb potential of the left-behind F₄TCNQ anions.

CPP 24.5 Wed 10:45 H40

Characteristics of the temperature dependent excitonic transport of organic semiconductors — ●A. K. TOPCZAK¹ and J. PFLAUM^{1,2} — ¹Exp. Phys. VI, University of Würzburg, D-97074 Würzburg — ²ZAE Bayern, D-97074 Würzburg

The excitonic transport in organic materials is described either by a temperature activated incoherent hopping model (polymers) or by a band-like coherent transport (single crystals) [1]. To gain insights into the respective behavior we performed temperature dependent Photoluminescence (PL) quenching measurements on the excitonic transport of the archetypical material C₆₀ and Diindenoperylene (DIP). The morphological thin film structure of these two materials differs substantially. Whereas C₆₀ is X-ray amorphous, DIP shows high crystalline order along the direction of exciton transport. By the PL quenching technique we obtained information of the temperature dependence of exciton diffusion and thereby on the related activation energies in correlation to the underlying film morphology. In the case of DIP we observed indication for a temperature independent exciton motion below 80 K and below a critical thickness of 80 nm. Together, this hints at a coherent exciton transport within the single crystalline domains of DIP and which becomes thermally activated if the exciton has to cross grain boundaries within the layer. This result emphasizes the importance of long range crystalline order to achieve maximum exciton harvesting in planar heterojunction photovoltaic cells and thereby to enhance their performance. Financial support by the DFG (project SPP1355). [1] P. Stallinga, *Adv. Mater.* 23 (2011) 3356-3362

CPP 24.6 Wed 11:00 H40

Unraveling the extraordinary conformational flexibility of poly(3-hexyl thiophene) by single-molecule spectroscopy — ●FLORIAN STEINER¹, JAN VOGELSANG^{1,3}, ALEX THIESSEN², TAKUJI ADACHI^{1,3}, and JOHN LUPTON^{1,2} — ¹Universität Regensburg — ²University of Utah — ³University of Texas at Austin

Poly(3-hexyl thiophene) (P3HT) has been used for many years for organic solar cells and field-effect transistors due to effective intermolecular selforganization in bulk films. It has been shown that the optical

properties strongly depend on the processing conditions. Using single-molecule spectroscopic techniques we are able to link the conformation of the P3HT chains embedded in a host matrix with their photophysical properties. We show that the conformation of a single polymer chain can be influenced by the polarity of the environment, which has been identified by measuring the excitation polarization dependence by wide-field fluorescence microscopy. Additionally, by performing confocal microscopy we could relate the conformation to specific fluorescence characteristics: an ordered conformation leads to a large red-shift of the fluorescence emission of more than 100 nm, accompanied by strong photon anti-bunching, longer fluorescence lifetime and a decrease of the fluorescence quantum yield as compared to a disordered conformation. The data clearly exemplifies the large conformational and spectroscopic variability of P3HT at the single molecule level. We propose that the vast unprecedented variability in single-chromophore transition energies actually drives selforganization in the solid, offering a challenge for future materials and device optimization.

15 min. break

CPP 24.7 Wed 11:30 H40

Molecular Ordering and Charge-Transport Properties of Semi-Crystalline Conjugated Polymers via Computer Simulations — ●CARL POELKING¹, EUNKYUNG CHO², ALEXANDER MALAFEEV³, VIKTOR IVANOV³, KURT KREMER¹, CHAD RISKO², JEAN-LUC BREDAS², and DENIS ANDRIENKO¹ — ¹Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — ²Center for Organic Photonics and Electronics, Georgia Institute of Technology, Atlanta, USA — ³Physics Department, Moscow State University, Moscow, Russia

We establish a link between the microscopic ordering, charge-transport parameters and carrier mobilities for semi-crystalline polymeric semiconductors using a computational multiscale approach. As material examples, we investigate poly(bithiophene-alt-thienothiophene) (PBTTT) and the polymorphic poly(3-hexyl-thiophene) (P3HT). We identify the structural origin of the regioregularity effect on mobility as a broadened energetic density of states and resolve how the packing of side chains, ranging from highly crystalline to amorphous, affects dynamics and distributions of site energies and electronic couplings via orthogonal modes of the backbone paracrystallinity. Simulated hole mobilities are in excellent agreement with experimental values for organic field-effect transistors. The results underline that to secure efficient charge transport in conjugated polymers, (i) electronic couplings should present fast dynamics next to high average values, and (ii) backbone paracrystallinity (intimately related with energetic disorder) should be small.

CPP 24.8 Wed 11:45 H40

Triplet state kinetics of anthracen studied by pulsed electron paramagnetic resonance — ●SILVIA DOMINGO KÖHLER, SEBASTIAN HÖFEL, and MALTE DRESCHER — Universität Konstanz, 78457 Konstanz, Germany

Photoexcited triplet states (total spin S = 1) of anthracen in a glassy toluene matrix were investigated using pulsed UV-laser photoexcitation and pulsed EPR spectroscopy. The optical spin polarization was studied time dependently resulting in the determination of the triplet lifetime and the triplet relaxation rates between the high-field eigenstates. The relative triplet state populations in zero-field and high-field are quantitatively analyzed. The kinetics of the triplet states were measured for different orientations of the molecule.

CPP 24.9 Wed 12:00 H40

Model systems for interchromophoric interactions in conjugated polymer materials — ●THOMAS STANGL¹, SEBASTIAN BANGE¹, DANIELA SCHMITZ², DOMINIK WÜRSCH¹, SIGURD HÖGER², JAN VOGELSANG¹, and JOHN M. LUPTON¹ — ¹Universität Regensburg, Regensburg, Deutschland — ²Universität Bonn, Bonn, Deutschland

A set of pi-conjugated oligomer dimers templated in molecular scaffolds is presented as a model system of the interactions between chromophores in conjugated polymers. Single-molecule spectroscopy was used to reveal energy transfer dynamics and electronic aggregation between two oligomers in either parallel conformation with different well-defined distances or oblique-angle geometry. First, it is concluded that the model systems presented here can be used to investigate the impact of H-aggregation as a function of interchromophoric distance by

lifetime and single-molecule spectral measurements. Second, the long-term non-equilibrium dynamics of energy transfer within the weakly coupled bichromophoric systems, however, is found to be accessible by studying the linear dichroism in emission at the single-molecule level, revealing reversible switching of the emission between the two oligomers. In bulk polymer films, strong and weak interchromophoric coupling impacts the functionality, e.g. the emission colour and the migration of excitation energy to quenching sites. Realizing the presence and dynamics of such interactions is crucial for understanding limitations in quantum efficiency of larger conjugated polymer materials.

CPP 24.10 Wed 12:15 H40

Probing charge carrier - exciton interactions in Diindenoperylene by the photoluminescence response of thin film transistors — ●N.H. HANSEN¹, C. WUNDERLICH¹, A.K. TOPCZAK^{1,2}, and J. PFLAUM^{1,3} — ¹Experimental Physics VI, Julius Maximilians University of Würzburg, 97074 Würzburg — ²Center for Nanosystems Chemistry, 97074 Würzburg — ³ZAE Bayern, 97074 Würzburg

Exciton loss mechanisms play a significant role in organic devices such as organic photo-voltaic cells (OPVs) or organic light emitting diodes (OLEDs). We present a novel approach to investigate the interplay between excitons and charge carriers by means of photoluminescence (PL) measurements on organic thin film transistors (OTFT). For this purpose, the organic semiconductor Diindenoperylene was utilized as active OTFT material. The OTFT geometry benefits from a spatially defined zone for the interaction between charges and photo-generated excitons leading to an intensity reduction of the DIP photoluminescence of up to 4.5%. This effect is found to correlate with the accumulated hole carrier density below the threshold voltage and provides access to the non-radiative exciton-hole recombination rate. Taking into account the respective measurement geometry, the estimated recombination rate of about $0.3 \cdot 10^{-10} \frac{cm^3}{s}$ compares sufficiently well with data reported on single crystals [1]. From the similarity of the threshold voltage and the saturation voltage above which the quenching becomes constant, we conclude the quenching process to be preferentially mediated by trapped holes within the DIP accumulation layer. [1] N. Wakayama and D.F. Williams, *J. Chem. Phys.*, 57(4):1770, 1972

CPP 24.11 Wed 12:30 H40

Particularities of Charge Carrier Localization in (DOEO)₄[HgBr₄].TCE Single Crystals — ●ALISA

CHERNENKAYA^{1,2}, KATERINA MEDJANIK¹, ALEKSANDR KOTOV², ANDREI GLOSKOVSKI³, OKSANA KOPLAK², EDUARD YAGUBSKI², GERD SCHÖNHENSE¹, and ROMAN MORGUNOV² — ¹Inst. für Physik, Univ. Mainz, Germany — ²Inst. of Problems of Chem. Phys., Rus. Acad. of Science, Russia — ³HASYLAB/DESY, Hamburg, Germany

The combination of classical conductivity measurements with electron spin resonance (ESR) spectroscopy, hard X-ray photoelectron spectroscopy (HAXPES, experiment has been performed at PETRA III (beamline P09)) and near edge X-ray absorption fine structure (NEXAFS) make it possible to characterize electronic processes around the critical temperatures in the organic charge transfer salts. We discuss the example of (DOEO)₄[HgBr₄].TCE that was studied by means of the methods mentioned above [1, 2]. It was found that the charge carrier localization begins at $T = 140$ K and at $T \leq 70$ K there is clear evidence of two types of centers. Electrons in the crystal give different signals below the critical temperatures: there is an additional line in ESR spectra, a sharp jump in the temperature dependence of SQUID data and shifts of core-level positions in the HAXPES spectra.

Funded via DFG (Transregio SFB TR49) and BMBF (05K 12 UM2).

[1] A. Bardin et al., *Coord.Chem.*, 32, 88 (2006)

[2] A. Chernenkaya et al., *Synth.Met.*, submitted

CPP 24.12 Wed 12:45 H40

Organic π -conjugated copolymers as molecular charge-qubits — ●CESAR AUGUSTO MUJICA MARTINEZ, PETER NALBACH, and MICHAEL THORWART — I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg, Deutschland

Organic π -conjugated polymers are systems that combine the electronic properties of semiconductors and the mechanical properties of plastics. Similar to their inorganic semiconductor heterostructures counterparts, it is possible to control the spatial degrees of freedom of charge carriers by constructing unimolecular organic heterostructures from π -conjugated block copolymers. We propose a design for molecular charge-qubits based on poly-(*p*-phenylene) and poly-diacetylene π -conjugated heterostructures and determine their electronic structure as well as their vibrational active modes. By tuning the length of the constituent oligomers, the tunnel coupling in the charge qubit and its decoherence properties due to molecular vibrations can be chemically engineered. Long coherence times are observed even when the qubit is operated at room temperature. It is found that the molecular vibrational spectrum induces strong non-Markovian electronic effects which support the survival of quantum coherence.

CPP 25: Biomaterials and Biopolymers II (joint session BP/CPP)

Time: Wednesday 9:30–12:45

Location: H43

Topical Talk

CPP 25.1 Wed 9:30 H43

Processing of recombinant proteins for biomaterials applications: about spider silk and more — ●THOMAS SCHEIBEL — Universität Bayreuth, Lehrstuhl Biomaterialien, 95440 Bayreuth, Germany

Proteins reflect one fascinating class of natural polymers with huge potential for technical as well as biomedical applications. One well-known example is spider silk, a protein fiber with excellent mechanical properties such as strength and toughness. During 400 million years of evolution spiders became outstanding silk producers. Most spider silks are used for building the web, which reflects an optimized trap for flying prey. We have developed biotechnological methods using bacteria as production hosts which produce structural proteins mimicking the natural ones. Besides the recombinant protein fabrication, we analyzed the natural assembly processes and we have developed spinning techniques to produce protein threads closely resembling natural silk fibers. In addition to fibers, we employ silk proteins in other application forms such as hydrogels, particles or films with tailored properties, which can be employed especially for biomaterials applications.

CPP 25.2 Wed 10:00 H43

Nano-confined protein anchors, structured by STED lithography, probed by dSTORM. — ●RICHARD WOLLHOFEN¹, MORITZ WIESBAUER^{1,2}, KURT SCHILCHER², JAROSLAW JACAK^{1,2}, and THOMAS A. KLAR¹ — ¹Johannes Kepler University, Linz, Austria — ²Upper Austria University of Applied Sciences, Linz, Austria

The ability to place individual proteins onto nano-confined struc-

tures plays a constantly growing role in bioscience, from basic studies in biology to development of nanosensors. One of the possibilities to generate sub-micrometer sized structures is direct laser writing (DLW) lithography. The resolution of DLW can be enhanced by stimulated emission depletion (STED) for assembly of polymeric structures down to several tens of nanometers [1]. Using a pulsed 780nm laser for two-photon DLW and a 532nm laser for STED, we are able to obtain structure sizes of down to 55nm and manufacture two clearly separated lines with 120nm distance [2]. The structures show good biocompatibility and allow an easy biofunctionalization with proteins down to the single protein level. We use direct stochastic optical reconstruction microscopy (dSTORM), which enables determination of protein density at a nanoscale level [3]. Combining STED lithography with dSTORM allows us to produce and characterize biocompatible structures, applicable to many biological assays. [1]J. Fischer et al., *Adv.Mat.*, Vol.22, Nr.32, pp.3578-3582(2010); [2]R. Wollhofen et al., submitted; [3]S. van de Linde et al., *Photochem.&Photobiol.Sc.*, Vol.8, Nr.4, pp.465-469(2009);

CPP 25.3 Wed 10:15 H43

Influence of direct laser written three-dimensional topographies on osteoblast-like cells — ●JUDITH K. HOHMANN¹, ERIK H. WALLER¹, RAINER WITTIG², RUDOLF STEINER², and GEORG VON FREYMAN¹ — ¹Physics Department and Research Center OPTIMAS, University of Kaiserslautern — ²Institute for Laser Technologies in Medicine and Metrology (ILM) at the University of Ulm

Biological cells react to various signals of their environment. While bio-

chemical pathways have been investigated for decades, the influence of physical characteristics of the cellular environment has only been studied in the very recent past [1]. Especially information on the interaction with three-dimensional structures is barely available, since common chemical and/or physical surface treatments (e.g. acid-etching, sand blasting) lead to randomly shaped surface topographies. In general, results generated in such two-dimensional systems can hardly be transferred to natural, three-dimensional conditions.

Our well-defined three-dimensional templates are fabricated by direct laser writing and coated with titanium dioxide via atomic layer deposition. This allows us to provide biocompatible substrates.

We aim at understanding the relation between various three-dimensional structures and viability parameters of osteoblastic cells. To observe cellular behavior, SaOs-2 osteosarcoma cells are seeded onto the structures in order to test proliferation, morphology, adhesion and differentiation via fluorescence and staining techniques. These results might lead to novel dental implant surfaces which promote osseointegration. [1]Nikkhah et al. *Biomaterials* 33 (2012) 5230-5246

CPP 25.4 Wed 10:30 H43

Biocompatibility of Fe-Pd ferromagnetic shape memory alloys - influence of surface roughness and protein coatings — ●UTA ALLENSTEIN^{1,2,3}, YANHONG MA², ARIYAN ARABI-HASHEMI², STEFAN G. MAYR^{2,3,4}, and MAREIKE ZINK¹ — ¹Division of Soft Matter Physics, Institute for Experimental Physics I, University of Leipzig — ²Leibniz-Institute for Surface Modifications (IOM) — ³Translational Center for Regenerative Medicine (TRM), University of Leipzig — ⁴Faculty of Physics and Earth Sciences, University of Leipzig

Recent decades have seen a huge turn in implantology and biomaterial development towards regenerative medicine. The approach in orthopedic surgery is no longer to just replace damaged tissue by a passive implant that evokes the least possible interference with biological tissue, but rather to provide active stimulation and actuation. Fe-Pd ferromagnetic shape memory alloys are a promising new class of smart materials with a unique set of properties ideal for biomedical applications, including superelasticity, magnetically switchable strains and biocompatibility. In this study the latter was shown by in vitro experiments with NIH 3T3 fibroblasts, MCF 10A epithelial cells and HOB osteoblasts on vapor-deposited single crystalline Fe₇₀Pd₃₀ thin films and roughness graded polycrystalline splat-quenched samples. Proliferation, adhesion and morphology were assessed on substrates of different surface roughness and different adhesive coatings, such as fibronectin, laminin and poly-L-lysine, as well as RGD peptides.

CPP 25.5 Wed 10:45 H43

Sorption of proteins to charged microgels: characterizing binding isotherms and driving forces — ●CEMIL YIGIT, NICOLE WELSCH, MATTHIAS BALLAUFF, and JOACHIM DZUBIELLA — Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, Hahn-Meitner Platz 1, 14109 Berlin, Germany

We present a set of Langmuir binding models in which electrostatic cooperativity effects to protein sorption is incorporated in the spirit of Guoy-Chapman-Stern models, where the global substrate (microgel) charge state is modified by bound reactants (charged proteins). Application of this approach to lysozyme sorption to oppositely charged core-shell microgels allows us to extract the intrinsic, binding affinity of the protein to the gel, which is salt-concentration independent and mostly hydrophobic in nature. The total binding affinity is found to be mainly electrostatic in nature, changes many orders of magnitude during the sorption process, and is significantly influenced by osmotic deswelling effects. The intrinsic binding affinity is determined to be about 7 kT for our system. We additionally show that Langmuir binding models and those based on excluded-volume interactions are formally equivalent for low to moderate protein packing, if the nature of the bound state is consistently defined. Having appreciated this, a more quantitative interpretation of binding isotherms in terms of separate physical interactions is possible in future for a wide variety of experimental approaches.

CPP 25.6 Wed 11:00 H43

Diffusion and Adsorption of Proteins in Mesoporous Environments — ●SEBASTIAN MÖRZ¹ and PATRICK HUBER² — ¹Experimental Physics, Saarland University — ²Materials Physics and Technology, Hamburg University of Technology

In the recent years, several studies discussed the encapsulation of biomolecules in mesoporous materials and its potential applications

in e.g. protein chromatography or as novel means of controlled drug release. Both the diffusion of biomolecules under such confinement and the interaction with the surface of the host material are crucial to these applications.

In this study, we examine the adsorption of bovine heart cytochrome c onto the pore surface of the porous silica material SBA-15. Comparison between the folded and unfolded state of this protein allows us to separate the contributions from the different interaction mechanisms involved i.e. coulombic and hydrophobic interaction. Furthermore, we attempt a qualitative validation of the Stokes-Einstein equation for the diffusion of proteins in a porous anodized aluminum oxide membrane and its applicability for protein separation.

15 min break

CPP 25.7 Wed 11:30 H43

FACS-sorting of particles to reduce the data variance in Optical Tweezers assisted Dynamic Force Spectroscopy measurements — ●TIM STANGNER¹, DAVID SINGER², CAROLIN WAGNER¹, CHRISTOF GUTSCHE¹, OLAF UEBERSCHÄR¹, RALF HOFFMANN², and FRIEDRICH KREMER¹ — ¹Universität Leipzig, Institut für Experimentelle Physik I, Linnéstraße 5, 04103 Leipzig, Deutschland — ²Biotechnologisch-Biomedizinisches Zentrum Leipzig, Fakultät für Chemie und Mineralogie, Deutscher Platz 5, 04103 Leipzig, Deutschland

By combining Optical Tweezers assisted dynamic force spectroscopy experiments with fluorescence activated cell sorting (FACS), we demonstrate a new approach to reduce the data variance in measuring receptor-ligand-interactions on a single molecule level by ensuring similar coating densities. Therefore, the carboxyfluorescein-labeled monophosphorylated peptide tau226-240[pThr231] is anchored on melamine resin beads and these beads are sorted by FACS to achieve a homogeneous surface coverage. To quantify the impact of the fluorescence dye on the bond parameters between the phosphorylated peptide and the corresponding phosphorylation specific anti-human tau monoclonal antibody HPT-104, we perform dynamic force spectroscopy and compare the results to data using unsorted beads covered with the non-fluorescence peptide analogue. Finally, we demonstrate that the data variance of the relative binding frequency is significantly decreased by a factor of 3.4 using presorted colloids with a homogeneous ligand coating compared to unsorted ones.

CPP 25.8 Wed 11:45 H43

Thermal vibrations reduce the efficacy of sacrificial bonds — ●SORAN NABAVI¹, MATTHEW J. HARRINGTON², PETER FRATZL², OSKAR PARIS¹, and MARKUS A. HARTMANN¹ — ¹Institute of Physics, Montanuniversität Leoben, Leoben, Austria — ²Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, Potsdam, Germany

Mussel byssal threads are a fascinating biological material combining high stiffness, toughness and extensibility. Experimental studies suggest that these outstanding properties are achieved by using so called sacrificial bonds (SBs) which are weaker than the covalent bonds holding the structure together and that can form and open reversibly [1]. The SBs break before the covalent bond rupture, providing hidden length and allowing for efficient energy dissipation.

In this study computer simulations are used to investigate the effect of SBs on the mechanical properties of a single polymeric chain. Special emphasis was put on the interplay of covalent and sacrificial bonds and the effect of thermal vibrations that have been largely overlooked in the description of SBs so far. In a simple setting with only one SB it is found that molecular chain fluctuations reduce the efficacy of SBs. Even for SBs with rather high binding energies of ~1 eV backbone fluctuations lead to a rupture of SBs before external loading sets in. Thus, the theoretical strength of SBs is reduced more than a factor of two. This effect increases with increasing polymeric chain length and with increasing temperature.

[1] M. J. Harrington et al., *J. Struct. Biol.* 167, 47 (2009)

CPP 25.9 Wed 12:00 H43

Benchmarking the water-peptide interaction — ●SUCISMITA CHUTIA, MARIANA ROSSI, and VOLKER BLUM — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin

The interaction between water molecules and the hydration sites of peptides is critical for any quantitative modeling of solvated peptides. We address this interaction for the successive hydration of two

peptides for which accurate experimental reference data exist: Ac-Ala₅-LysH⁺ (non-helical) and Ac-Ala₈-LysH⁺ (helical). In particular, finite-temperature Gibbs reference water binding energies ΔG_0 and equilibrium constants are known [1,2]. However, earlier force-field predicted preferred water binding sites do not agree with one another. We present an exhaustive first-principles study (density-functional theory based on the van der Waals corrected PBE functional) that demonstrates [3]: (i) There is a close competition between possible hydration sites (protonated carboxyl group or ammonium group). The preferred first hydration site breaks an intramolecular bond of the ammonium group in the unsolvated molecule. (ii) Calculated $\Delta G_0(T)$ are in remarkable agreement with experimental data. Lowest-energy H₂O H-bond networks are predicted for up to five H₂O molecules, and the connection to the solvated state is explored by ab initio molecular dynamics with up to 152 H₂O molecules. [1] Liu, Wyttenbach, Bowers, *IJMS*. 236, 81 (2004) [2] Kohtani, Jarrold, *JACS*. 126, 8454 (2004) [3] Chutia, Rossi, Blum, *JPCB* DOI: 10.1021/jp3098268

CPP 25.10 Wed 12:15 H43

Biomolecular translocation through nanopores: from statistics to real DNA conformations — ●MARIA FYTA¹, SIMONE MELCHIONNA², SAURO SUCCI³, and EFTHIMIOS KAXIRAS⁴ — ¹Institut für Computerphysik, Universität Stuttgart, Germany — ²IPCF-CNR, Università La Sapienza, P.le A. Moro 2, 00185 Rome, Italy — ³IAC-CNR, Via dei Taurini 19, 00185 Rome Italy — ⁴Department of Physics and School of Engineering and Applied Sciences, Harvard University, Cambridge MA 02138, U.S.A

We apply a multiscale computational scheme to model a biomolecule translocating through a narrow pore, an intensively studied subject due to its variety of applications such as ultra-fast DNA sequencing. The model uses a mesoscopic lattice Boltzmann method to treat the solvent and a Molecular Dynamics scheme to deal with the biomolecule. Our

first results involve an anonymous polymer translocating in pure water. We have obtained important insight into the statistics and dynamics of the process. The translocation time exponent compares well with the experimental values, while we were able to monitor multiconformational translocation. As a next step, we include electrokinetic effects, i.e. ions, as well as a realistic quantum-mechanically derived potential for double stranded DNA. We are now able to reveal in more detail the structural conformations of the DNA molecule as well as the ion distribution within the pore. The results also provide a qualitative and quantitative understanding of the ionic conductance and DNA blockade as compared to the experiments. Our conclusions also involve the effect of the pore geometry in the DNA translocation process.

CPP 25.11 Wed 12:30 H43

Driving forces in corneocyte expansion: a geometric perspective — ●MYFANWY EVANS¹ and ROLAND ROTH² — ¹Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Deutschland — ²Theoretische Physik, Universität Tübingen, Deutschland

The arrangement of keratin in corneocytes, the dead cells in the outer layer of mammalian skin, are likely a highly ordered packing of helical filaments. This specific geometric arrangement allows the exotic physical property of cell expansion on prolonged exposure to water to occur in a mechanically stable and reversible regime. We examine the solvation free energy of a water-like solvent filling the volume of the corneocytes around the hydrophilic keratin fibres by the morphometric approach to energy landscapes. We find that the energy minimisation drives the system to absorb water and expand where water is available. During this expansion, the elastic energy in the keratin intermediate filaments increases, and the balance of the two forces forms a natural limit for the expansion process and the system maintain full reversibility.

CPP 26: Focus: Wetting on smooth and rough surfaces: From spreading to superhydrophobicity II

Wetting determines the morphology and dynamics of a liquid on a surface. In particular for rough, structured, or deformable surfaces the dynamic contact angles are poorly understood. Progress in experimental and numerical techniques permit time resolved three-dimensional investigations of wetting, providing new insight into the interplay between the contact angle, hysteresis, and pinning.

Organizers: Hans-Jürgen Butt (Mainz), Stephan Herminghaus (Göttingen), Doris Vollmer (Mainz)

Time: Wednesday 15:00–16:30

Location: H34

Invited Talk CPP 26.1 Wed 15:00 H34
Leidenfrost Dynamics — ●DAVID QUÉRÉ — ESPCI & Ecole polytechnique, Paris

We discuss the Leidenfrost phenomenon, and particularly focus on its dynamical aspects: how can liquids levitate on a hot solid? what are their particular shape and evolution? what is the friction of these liquid hovercrafts when they move? how do they behave on an irregular solid? is it possible to create a Leidenfrost situation without heat? We'll see that the absence of contact between a substrate and a liquid deeply modifies the usual laws of wetting.

CPP 26.2 Wed 15:30 H34

Directed motion of droplets on asymmetrically structured vibrating substrates: a Molecular Dynamics study — ●NIKITA TRETYAKOV and MARCUS MÜLLER — University of Göttingen

We study a transport of coarse-grained polymer droplets on asymmetrically structured (sawtooth shaped) and vibrating substrates by means of Molecular Dynamics. The temperature of the system is controlled by the DPD thermostat. Due to a continuous supply of power by substrate vibrations and the asymmetry of its topography, the droplets are driven in a preferred direction. This directed motion is investigated as a function of the size of the droplets, linear dimension of the substrate corrugation and the period of substrate vibrations. To this end, our main concern consists in resolving two questions: (i) what is the driving mechanism and (ii) what is the character of the flow inside the droplet?

A typical mechanism of driving is the one provided by droplet's contact lines, as the responses of the advancing and receding contact lines on the vibrating asymmetric substrate are not identical. We, moreover,

find a range of vibration periods that lead to an additional driving by the contact area of the substrate between the contact lines.

For the character of the droplet motion there are, in general, three possibilities: sliding, rotating and a combination of both. All of them dissipate the input power by different means. We find that for most of the parameters the droplets are sliding, but the linear size of the substrate corrugation may give a rise to an additional rotation.

CPP 26.3 Wed 15:45 H34

Trapping and release of drops by electrically tunable wetting defects — DIETER 'T MANNETJE¹, RUDY LAGRAAUW¹, SIMON OTTEN¹, ARUN BANPURKAR^{1,2}, ARJEN PIT¹, DIRK VAN DEN ENDE¹, and ●FRIEDER MUGELE¹ — ¹University of Twente, Physics of Complex Fluids, MESA+ institute for Nanotechnology, Enschede, The Netherlands — ²University of Pune, Department of Physics, Pune, India

Drops driven across heterogeneous by gravity, viscous drag, and air flow can get stuck at pinning sites that are sufficiently strong compared to the external driving force. Using defects of continuously variable strength generated by electrowetting we study the critical conditions required to pin and depin drops of sliding down an inclined plane. We show that the strength of the electrical defects scales with the square of the applied voltage and with the radius of the drop. A generalized model incorporating the variable strength of the defect, viscous dissipation, and inertia of the sliding drop provides a general pinning criterion in excellent agreement with the experiments. We demonstrate the potential of electrically tunable defects as tools to manipulate and guide drops on inclined planes and in microfluidic devices.

CPP 26.4 Wed 16:00 H34

Wetting of non regular rough 3D surfaces — ●CIRO SEMPREBON, STEPHAN HERMINGHAUS, and MARTIN BRINKMANN — MPI-DS, Göttingen, Germany

Modelling wetting of disordered rough surfaces is a challenging problem as the liquid interface can adopt a large number of different topologies in mechanical equilibrium. A recent study of regular surface topographies demonstrates that topological changes of the interface are important to understand the variety of emerging advancing and receding contact angles [1]. Here, we present a method to compute interfacial equilibria on arbitrary substrate topographies while allowing for varying interface topology. In this method the material contact angle can be controlled via a short ranged interface potential. To demonstrate its applicability, we studied drying of a rough substrate while decreasing the Laplace pressure of the wetting film. The results are compared to drying during a decrease of the total liquid volume or an increasing material contact angle at fixed Laplace pressure.

CPP 26.5 Wed 16:15 H34

Understanding the behaviour of super-cooled liquid on nanostructured surfaces: A molecular dynamics study — JAYANT

SINGH^{1,2} and ●FLORIAN MÜLLER-PLATHE¹ — ¹Technische Universität Darmstadt, Theoretical Physical Chemistry, Petersenstr. 22, 64287 Darmstadt — ²Department of Chemical Engineering, Indian Institute of Technology Kanpur, Kanpur, India -208016, India

Understand the role of roughness of the surface in suppressing the ice formation is of critical importance in the design of ice-free nanostructured surfaces. While recent work has provided some insight to the design of superhydrophobic surfaces for deicing applications, yet it is not clear that having roughness leading to hydrophobicity itself is good enough for the smart design of ice-free nanostructure surface.

In this work, using extensive molecular dynamics we have investigated the behaviour of super cooled water on smooth and rough surfaces. Roughnesses of the order of 1-2 nm were created on graphite like surfaces. Water is modeled as monatomic water model. In particular, we investigate the role of surface fraction (fraction of solid on the interface) and roughness on the onset of crystallization while cooling from 270 K to 190 K with a cooling rate of 0.5-1K/ns. We also present in detail ice cluster growth and ice phases as observed for different rough surfaces.

CPP 27: Nanoparticles and Composite Materials II

Time: Wednesday 15:00–16:30

Location: H39

CPP 27.1 Wed 15:00 H39

Growth of silver nanowires within nanotubular J-Aggregates — ●EGON STEEG, HOLM KIRMSE, FRANK POLZER, YAN QIAO, JÜRGEN RABE, and STEFAN KIRSTEIN — Institut für Physik, Humboldt-Universität zu Berlin

It was demonstrated earlier [1] that ultrathin but long Ag nanowires with diameters less than 7 nanometer and length exceeding micrometers can be fabricated by reduction of silver salt using uniform nanotubular J-Aggregates of amphiphilic cyanine dyes as templates. Here, we report on the growth mechanism of these Ag wires as revealed by conventional and cryogenic transmission electron microscopy. The growth is initiated by short illumination with UV light and observed over time scales ranging from minutes to days. In an early stage, within the tubular aggregates silver nanoparticles are formed which act as seeds for continuous growth of separate pieces of wires. The diameter of the wires is determined by the inner diameter of the tubes. In the final state, the pieces of wire totally fill the aggregate. As revealed by high resolution TEM, the fragmented growth of the wires from separate seeds leads to silver nanowires consisting of single crystalline domains exceeding 100 nm in length. The growth process indicates transport of Ag-ions through the tubular wall membrane. The experiments demonstrate that these J-aggregates may also act as a soft template for the growth of other wire-like inorganic materials.

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

CPP 27.2 Wed 15:15 H39

Adhesion Forces between TiO₂ Nanoparticles in Agglomerates — ●REBECCA SCHOLZ¹, SAMIR SALAMEH², and LUTZ MÄDLER² — ¹Ruhr-Universität Bochum, Physical Chemistry I, Universitätsstraße 150, 44801 Bochum — ²Foundation Institute of Materials Science (IWT), Department of Production Engineering, University of Bremen, Badgasteiner Str. 3, 28359 Bremen

Nanoparticle aggregates and their films have wide spread applications such as catalysis, sensing, and hybrid materials. The adhesion force between the aggregates plays a major role for their functionality and influence mechanical but also chemical stability. Therefore, information on key parameters influencing the particle-particle-contact are very important. However, direct measurements of the contact forces for particles in size ranges of about 10 nm are rather challenging. Here, we present a method to determine these forces [1], which includes a statistical analysis of the force curves measured by atomic force microscopy (AFM) and in-situ measurements of the rearrangements of the nanoparticles in an AFM/TEM setup. We use this method to first clarify the question of the influence of the primary TiO₂ particle size on the contact force and to then investigate the agglomerate size. In order to separate the influence of the agglomerate size we generated monodisperse agglomerates. Our results show that sliding and rolling events increase with agglomerate size. These findings, especially of the influence of the agglomerate size on the contact force, will be presented

and discussed in this presentation.

CPP 27.3 Wed 15:30 H39

Fluorescence spectroscopy of individual semiconductor nanocrystals in solution — ●SANDRA FLESSAU and ALF MEWS — Institute for Physical Chemistry, University of Hamburg

Colloidal II-VI semiconductor nanocrystals are crystalline fragments of the corresponding bulk material with sizes of 1 to 10 nm. In this range, the surface-to-volume ratio is considerably large. For a CdSe nanocrystal of 3 nm in diameter, already one third of its atoms is at the surface. The states of the surface influence charge carriers which are three-dimensionally confined within this volume, and therefore become important in determining many of the nanocrystal properties like fluorescence intensity, fluorescence lifetime and blinking behavior.

Here, we present experiments on the impact of chemical or physical modification of the surface on individual nanocrystals. Therefore, the nanocrystals are immobilized within microfluidic channels which are fabricated by soft lithography. Time-resolved single particle fluorescence spectroscopy is performed to explore the details of photophysical changes of one and the same nanocrystal before and after rinsing the channel with varying solutions, e.g. with different dielectric properties or which contain different molecules that can attach to the nanocrystal surface.

CPP 27.4 Wed 15:45 H39

Electrochemical Manipulation of Single CdSe/ZnS Quantum Dots — ●NICOLE AMECKE, DAVID PLOTZKI, and FRANK CICHOS — Molecular Nanophotonics Group, University of Leipzig

Despite immense research on semiconductor quantum dots (QDs), the mechanisms of their intensity fluctuations remain a highly speculative subject. Most fluctuations are attributed to non-radiative decay channels arising from charges and fluctuating trap states at the QD interface, surface or close environment. A more specific assignment is difficult, especially due to the extraordinary statistics, which resemble power law distributions of bright and dark periods over several decades in time. With electrochemistry we can access those trap states as well as charges, while simultaneously monitoring QD intensity, lifetime and spectra. In this way we can observe the influence of reduction and oxidation processes on the fluorescence of each single QD. We find, that there is a preferred electrochemical potential for QD-fluorescence. Lower potentials introduce electrons in the conduction band, while higher potentials introduce trap states for the electron. The desired potentials depend on substrate, QD size and vary from dot to dot. The time dependence of the reaction to a potential step indicates a rearrangement of traps and charges in the QD environment.

CPP 27.5 Wed 16:00 H39

New Tools for reliable photoluminescence quantum yield measurements of near-infrared emissive quantum dots — ●SOHEIL HATAMI¹, SUSANNE LEUBNER², VLADIMIR LESNYAK², NIKO-

LAI GAPONIK², CHRISTAN WÜRTH¹, MARKUS GRABOLLE¹, ALEXANDER EYCHMÜLLER², and UTE RESCH-GENGER¹ — ¹BAM Federal Institute for Materials Research and Testing, Berlin, Germany — ²Physical Chemistry/Electrochemistry, TU Dresden, Dresden, Germany

Semiconductor quantum dots (QDs) are applied as fluorescent labels and active components in optical devices. QDs emitting in the near-infrared (NIR) region like CdTe, and CdHgTe are of increasing importance, due to their high photoluminescence quantum yields (QY) compared to any other chromophore at wavelengths above 900 nm. The characterization of the performance of these NIR and IR QDs requires reliable methods for the determination of QY under biological application-relevant conditions. For often performed relative optical measurements, standard dyes with precisely known QY are mandatory, with the lack of reliably assessed QY standards for the NIR hampering the performance of such measurements. This encouraged us to design a new integrating sphere setup for the absolute measurement of QY values in the spectral range of 600 nm to 1700 nm and to develop procedures for the relative and absolute determination of QY of emissive materials in this wavelength region. Here, the design of our setup and its calibration will be presented as well as first QY measurement of NIR dyes and CdTeHg QDs of varying size and material composition.

CPP 27.6 Wed 16:15 H39

CPP 28: Crystallization, Nucleation and Self Assembly II

Time: Wednesday 15:00–16:30

Location: H40

Invited Talk

CPP 28.1 Wed 15:00 H40

Self Organization of Colloidal Crystals and of Co-operative Propulsion by Salt Gradient Induced Flows — •THOMAS PALBERG — Inst. of Physics, Johannes Gutenberg Univ., Mainz, Germany

Colloidal crystallization from a meta-stable colloidal melt has been extensively studied with optical techniques. Most studies of charged colloidal spheres in aqueous suspension, were performed at low and homogeneous salt concentrations in a quiescent solvent. Recently we focused on the influence of salt gradients on the formation of crystals and their micro-structure. Gradients were obtained from a granular, electrolyte releasing particle settled under gravity onto the charged substrate. Depending on the electrolyte chosen and the charge sign of the substrate, strong, radially symmetric solvent flow is induced along the substrate, either towards or away from the granule. Release of HCl combined with an anionic substrate leads to a convergent flow. We use this flow to assemble micron sized colloidal particles sedimented to the substrate and swept towards the granule. Crystal formation kinetics are well understood in a simple theoretical model. Emerging micro-structures are well reproducible. An equivalent behavior is also seen in three dimensions. Together this offers a flexible way to manipulate and pattern the micro-structure of colloidal solids, which may be useful for the fabrication of photonics related materials. Very recently we observed that beyond the self organization of structures, the flow patterns may also be useful to self organize the linear propulsion of the granule-colloid complex. This possibly offers an alternative approach to swimming at low Reynolds numbers

CPP 28.2 Wed 15:30 H40

Self-Assembly of Janus-particles in critical fluids — •MARCEL LABBÉ-LAURENT^{1,2}, MATTHIAS TRÖNDLE^{1,2}, LUDGER HARNAU^{1,2}, and SIEGFRIED DIETRICH^{1,2} — ¹Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany — ²Universität Stuttgart, Germany

Critical fluctuations in simple fluids or binary liquid mixtures give rise to forces acting on immersed colloidal particles. These Casimir-like forces are attractive or repulsive depending on the chemical surface properties [1]. Spatial ordering of colloids opposite to chemically structured surfaces, induced by the critical Casimir effect, is observed experimentally for colloidal particles immersed in a critical water-2,6-lutidine mixture and is in agreement with theory [2]. Janus-particles immersed in a critical fluid are subject to orientation-dependent stabilizing and destabilizing forces. Within density functional theory we study the phase diagram of cylindrical and spherical Janus-particles. We find first and second order phase transitions between isotropic and structured colloidal phases. Janus-particles self-assemble into a doublelayer phase, which is tunable by temperature, density and external

Absolute Photoluminescence Quantum Yield of Hexagonal β -NaYF₄:Er³⁺, Yb³⁺ Upconversion Nanoparticles — •MARTIN KAISER¹, WÜRTH CHRISTIAN¹, RESCH-GENGER UTE¹, HYPÄNEN IKO², and SOUKKA TERO² — ¹BAM Bundesanstalt für Materialforschung und -prüfung, Richard-Willstätter-Str. 11, 12489 Berlin — ²Department of Biotechnology, University of Turku, Tykistökatu 6A, FI-20520 Turku, Finland

Hexagonal β -NaYF₄ doped with Er³⁺ and Yb³⁺ is currently the most efficient upconversion (UC) phosphor to convert near-infrared (NIR) to green light. For the design of nm-sized UC particles, there is a need for reliable spectroscopic tools for the characterization of the signal-relevant optical properties of these materials like the absolute quantum yield (QY), which equals the ratio of emitted to absorbed photons. Due to the upconverting nature of the photoluminescence and the lack of UC QY standards and conventional QY standards with absorption at 980 nm, the QY of these particles can be presently measured only absolutely. This presents a considerable challenge due to the low absorption coefficient of these materials and the power density dependence of QY. We present here a custom-designed integration sphere setup equipped with a power-stabilized 980 nm-laser diode for spectrally resolved and power density-dependent measurements of the absolute UC QY as well as the transmission and reflection of UC materials in suspension and in the solid state. The characterization of this setup is detailed as well as first QY of nm-sized β -NaYF₄:Er³⁺, Yb³⁺ in different environments.

potentials.

[1] C. Hertlein, L. Helden, A. Gambassi, S. Dietrich, and C. Bechinger, *Nature* **451**, 172 (2008).

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

CPP 28.3 Wed 15:45 H40

Heterogeneous Nucleation in colloidal melts at periodically structured substrates — •ACHIM LEDERER¹ and HANS JOACHIM SCHÖPE² — ¹Johannes Gutenberg Universität, Mainz, Germany — ²Max Planck Institut für Polymerforschung, Mainz, Germany

Monodisperse suspensions of colloidal spheres with known interaction are a terrific model system for testing predictions by statistical physics. Their typical length scales are accessible via optical methods like light scattering in reciprocal and microscopy in real space. We investigate heterogeneous nucleation and the microstructure evolution of colloidal model systems with hard sphere like behavior by Confocal Laser Scanning Microscopy (CLSM) observing local parameters on a single particle scale. In our studies we observe heterogeneous nucleation at fcc(111) patterned substrates as function of lattice spacing. By analyzing local order parameters we locate crystalline particles in clusters, determining cluster sizes and shape during nucleation and growth. By varying the lattice spacing we observe a transition from a commensurable to an incommensurable situation.

CPP 28.4 Wed 16:00 H40

Nanoparticle Assembly in a modular Fluidic System — •DOMINIK GERSTNER, PHILIP BORN, and TOBIAS KRAUS — Leibniz-Institut für Neue Materialien (INM), Campus D2.2, 66123 Saarbrücken

Nanoparticles are widely used in industrial and research applications. Agglomeration occurs in most use cases. We investigate structure formation during agglomeration to find which mechanisms govern the morphology of the agglomerates. For alkylthiol-stabilized gold nanoparticles with 6 nm core diameter, we found that the morphology depends crucially on the exact behavior of the ligand monolayer. Crystalline agglomerates only formed for a molten monolayer. Based on this study, we suggest that the particles' microscopic packing is dominated by contact mechanics rather than colloidal interactions [1].

The ligands' directing effect may be partially kinetic. We will discuss experiments to study agglomeration under defined mixing conditions and for different ligands efficiently. A modular fluidic system enables the preparation and direct observation of agglomerating nanoparticles in flow. Nanoparticle dispersion and agglomeration agent are merged in a micromixer. UV/Vis spectrometers or Light Scattering detectors subsequently provide characteristics of the growing agglomerates. The

versatility of the setup allows rapid experimentation with a wide range of particles and conditions. Correlation of spectroscopic and real-space TEM data yields a detailed understanding of agglomerate morphologies. We use it to search for ligands that lead to agglomerates with predictable morphologies applicable in hybrid materials.

[1] T. GEYER et al. *Phys. Rev. Lett.* 109 (2012), 128302.

CPP 28.5 Wed 16:15 H40

Free energy and concentration of thermal vacancies in closed-packing solids — ●MOSTAFA MORTAZAVIFAR, MOHAMMAD HOSSEIN YAMANI, and MARTIN OETTEL — Institut für Angewandte Physik, Eberhard Karls University of Tübingen, Tübingen, Germany

The free energy and the equilibrium concentration of thermally excited

vacancies in crystals has been studied since long ago using simulations in classical statistical mechanics or theoretical considerations on the phonon spectrum in the solid with vacancies. Here, we present a simple estimate of the vacancy free energy and concentration in close-packing solids using the leading-order term in an expansion in correlated free particles in a frozen, crystalline matrix [1]. For hard spheres, results are in excellent agreement with available simulation data, and have an intuitive interpretation in terms of available volumes of a free particle in the frozen matrix either next to a vacancy or in a perfect, crystalline surrounding. For solids of atoms interacting with soft potentials, computations can be easily done for broad ranges of temperature and density. We present results for the Lennard-Jones system and compare to available data from simulation and other theory.

[1] Stillinger et al, *J. Chem. Phys.* 43, 932 (1965).

CPP 29: Organic Electronics and Photovoltaics III (joint session O/CPP/DS/HL)

Time: Wednesday 16:00–19:00

Location: H33

CPP 29.1 Wed 16:00 H33

Effects of nuclear dynamics on light absorption, charge injection, recombination, and dye regeneration conditions in dye-sensitized solar cells — ●SERGEI MANZHOS¹, HIROSHI SEGAWA², and KOICHI YAMASHITA³ — ¹Department of Mechanical Engineering, National University of Singapore, Blk EA #07-08, Singapore 117576 — ²RCAST, University of Tokyo, 4-6-1, Komaba, Meguro-ku, Tokyo 153-8904, Japan — ³Department of Chemical System Engineering, University of Tokyo, 7-3-1, Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

We present molecular dynamics studies of effects of nuclear motions on light absorption and charge injection, recombination, and dye regeneration conditions for two organic dyes adsorbed on anatase (101) surface of TiO₂ in mono- and bi-dentate configurations. We studied the effects of temperature, deuteration, and co-adsorbed water. Averaged over nuclear motions driving forces for injection and regeneration can differ significantly from their static estimates computed in most works. As a result, injection rate could be different by orders of magnitude. As the expectation value of the ground state energy is higher than its optimum geometry value (by up to 0.1 eV), nuclear motions will affect dye regeneration by recently proposed redox shuttle-dye combinations operating at low driving forces. Dye orientation motions are predicted to increase back-donation rate by orders of magnitude. Dye structure, adsorption mode, and the presence of water affect strongly the dynamics of energy level matching. Temperature in the range of 300-350K and deuteration have little effect on driving forces but red-shift of the absorption spectrum by a few %.

CPP 29.2 Wed 16:15 H33

Photoemission Studies of Highly Reactive Organic Photosensitizers — ●MATHIAS FINGERLE¹, MAXIMILIAN HEMGESBERG², YVONNE SCHMITT², SEBASTIAN SCHMITT², DIMITRI IMANBAEW², HARALD KELM², EUGEN RISTO², STEFAN LACH¹, MARKUS GERHARDS², CHRISTOPH VAN WÜLLEN², WERNER THIEL², and CHRISTIANE ZIEGLER¹ — ¹Fachbereich Physik, Erwin-Schrödinger-Str. 56, D-67663 Kaiserslautern, Germany — ²Fachbereich Chemie, Erwin-Schrödinger-Str. 52, D-67663 Kaiserslautern, Germany

Substituted phenothiazines (PTs) are promising candidates for applications in the field of organic electronics. Due to the fact, that the electronic, magnetic and geometrical properties of the phenothiazine compared to its radical cation differ substantially, PT redox couples are of great interest for organic devices like dye sensitized solar cells (DSSCs). Here, the electronic properties of N-substituted phenothiazine dyes derived from 3,8-dithien-2-ylphenothiazine (DTPT), among them the first PT containing an olefinic moiety with an electron withdrawing group close to the nitrogen atom, were probed via photoemission spectroscopy. The thin film growth of the dyes and their oxidized species after spin coating was analyzed by X-ray photoelectron spectroscopy (XPS) and qualitatively visualized by scanning force microscopy (SFM). Through UV-photoelectron spectroscopy (UPS) and inverse photoelectron spectroscopy (IPES), the occupied and unoccupied energy levels could be attained and compared to data acquired by UV/Vis spectroscopy and DFT calculations. It is shown, that chemical oxidation by NOBF₄ leads to a dramatic decrease of the band gap.

CPP 29.3 Wed 16:30 H33

Investigation of the electronic structure of phosphorescent

Platinum(II) complexes on Au(111) by STM and STS — ●PASCAL RAPHAEL EWEN, HASMIK HARUTYUNYAN, JAN SANNING, MATTEO MAURO, CRISTIAN ALEJANDRO STRASSERT, and DANIEL WEGNER — Physikalisches Institut - Westfälische Wilhelms Universität Münster

Quenching effects still limit the efficiency of state-of-the-art organic light emitting diodes (OLEDs) at higher doping concentrations of the triplet emitter molecules within the emission layer. A possible candidate for avoiding of the loss of luminescence are recently synthesized Pt(II) complexes that do not show quenching even when aggregated into fibers or gels. The efficient implementation of such complexes in electronic devices requires a fundamental understanding of the interaction of the molecules with the local environment. A systematic investigation of the adsorption and the electronic structure of slightly different phosphorescent Pt(II) complexes offers information about the influence of ligands and substituents on the complexes as well as their interactions with neighbours and the substrate. We have studied the impact of molecule-surface and intermolecular interactions on the self-assembly and electronic structure of Pt-complex monolayers on Au(111) using scanning tunneling microscopy (STM) and spectroscopy (STS) at low temperature. By determining energies and spatial distributions of several frontier orbitals, we are able to evaluate the impact of hybridization on the molecular electronic structure with important consequences for the optical properties.

CPP 29.4 Wed 16:45 H33

Overcoming the limitations of work-function modifications induced by adsorption of self-assembled monolayers — ●OLIVER T. HOFMANN, YONG XU, PATRICK RINKE, and MATTHIAS SCHEFFLER — Fritz-Haber Institut der MPG, Berlin, Germany

Controlling the work function of electrodes critically determines charge-injection barriers and is of high importance for organic electronic devices. Such control can be easily achieved by adsorbing dipolar self-assembled monolayers. Despite the common application of this method, its limitations remain largely unexplored. It has, however, been demonstrated that charge-transfer occurs as soon as the molecular LUMO comes into resonance with the Fermi-energy when the molecular dipole moment is systematically increased by adding multiple repeat units. This Fermi-level pinning limits the achievable work-function modification. In turn, we argue that molecules with negative electron affinities never reach this limit and can reduce the work-function in principle all the way down to zero. As a proof of concept, we study the interaction between the ZnO(10 $\bar{1}$ 0) surface and pyridine using hybrid density functional theory with a variable fraction of exact exchange and a correction scheme for screened van-der-Waals forces. In agreement with experimental observations, we find an adsorption-induced work-function reduction of up to -2.9 eV. For a hypothetical ultra-dense pyridine monolayer the work-function reduction could even reach -4.3 eV for this surface.

CPP 29.5 Wed 17:00 H33

Surface electronic structure and electron dynamics for pristine and adsorbate-covered ZnO(10 $\bar{1}$ 0) — ●JAN-CHRISTOPH DEINERT, DANIEL WEGKAMP, MICHAEL MEYER, JULIA STÄHLER, and MARTIN WOLF — Fritz-Haber-Institut der MPG, Abt. Physikalisches Chemie, Faradayweg 4-6, 14195 Berlin

Zinc oxide is a promising electrode material for organic optoelectronics, because of its large optical band gap, possible n-type conductivity and its abundance. Despite many years of research, the electronic structure of interfaces between ZnO and - possibly functional - molecules or even its vacuum interface are not well understood. We use femtosecond time- and angle-resolved two-photon photoemission spectroscopy (2PPE) to analyze both the occupied and unoccupied electronic states and dynamics at such interfaces. We show that hydrogen adsorption, even for very low coverage, leads to the formation of a surface electron accumulation layer and thus surface metallicity. Above band gap excitation with 3.8 eV fs laser pulses leads to ultrafast relaxation of hot electrons in the ZnO(10 $\bar{1}$ 0) conduction band and the alleged formation of an excitonic state with a lifetime in the 100 ps range. Furthermore, we demonstrate that molecules with negative electron affinity allow for massive work function reduction of ZnO(10 $\bar{1}$ 0), e.g. by $\Delta\Phi = -2.9$ eV in the case of a monolayer of pyridine. This opens a pathway to the design of cathodes with optimal electron injection barriers. We furthermore examine the changes in interfacial electronic structure upon biphenyl adsorption, which serves as a model system for optoelectronically functional poly(*p*-phenylene)-type molecules.

CPP 29.6 Wed 17:15 H33

Defect-Driven Interfacial Electronic Structure at a Hybrid Organic / Inorganic Heterojunction — ●OLIVER MONTI¹, LEAH KELLY¹, LAURA SCHIRRA¹, PAUL WINGET², HONG LI², and JEAN-LUC BREDAS² — ¹The University of Arizona, Tucson, AZ, USA — ²Gregoria Institute of Technology, Atlanta, GA, USA

We present a combined experimental and theoretical study of the interfacial electronic structure of highly defined thin films of organic semiconductors on ZnO. We discuss the importance of shallow donor states in the near-surface region of ZnO in determining energy-level alignment and electronic structure at such interfaces. Using ultraviolet and x-ray photoelectron spectroscopy together with two-photon photoemission and first-principles calculations we investigate the nature of hybrid interface states inside the bandgap of ZnO. These states display strong charge-transfer character and may play an important role in charge-harvesting events in organic photovoltaic cells.

CPP 29.7 Wed 17:30 H33

Electronic structure and excited states dynamics in polythiophene — ●LEA BOGNER¹, GAURAV GUPTA², MICHAEL SOMMER³, MUKUNDAN THELAKKAT⁴, THOMAS THURN-ALBRECHT², and PETRA TEGEDER^{1,5} — ¹Freie Universität Berlin, Fachbereich Physik — ²Martin-Luther-Universität Halle-Wittenberg, Institut für Physik — ³Albert-Ludwigs-Universität Freiburg, Institut für Makromolekulare Chemie — ⁴Universität Bayreuth, Makromolekulare Chemie I — ⁵Rubrecht-Karls-Universität Heidelberg, Physikalisch-Chemisches Institut

Semiconducting conjugated polymers exhibit promising properties for applications in optoelectronic devices such as organic photovoltaic cells. Poly(3-hexylthiophene) (P3HT) and other poly- and oligothiophenes are auspicious electron donor materials due to their high charge carrier mobility. In this study thin films of semi crystalline P3HT with different degree of crystallinity [1] have been investigated by means of time- and angle-resolved two-photon photoemission (2PPE). We observed several unoccupied and occupied electronic states (bands) including the valence and conduction band. In addition two excited states are found which possess lifetimes in the order of hundred picoseconds.

Ref.: [1] Z. Wu, A. Petzold, T. Henze, T. Thurn-Albrecht, R. H. Lohwasser, M. Sommer, M. Thelakkat, *Macromolecules*, 2010, 43, 4646-4653.

CPP 29.8 Wed 17:45 H33

Charge transfer at the interface between substituted pentacene nanorods and gold single crystals — ●SABINE-ANTONIA SAVU, MARIA BENEDETTA CASU, and THOMAS CHASSÉ — Institute of Physical and Theoretical Chemistry, University of Tübingen, Tübingen, Germany

Pentacene is one of the most investigated organic molecules due to its successful application in organic electronics. Substitution in pentacene gives the opportunity to tailor the properties which are needed for applications; therefore it is necessary to investigate its influence on molecular aggregation and thin film formation. In particular, here we report our investigations on nanorods of three newly synthesized substituted pentacenes with different degrees of fluorination. We performed X-ray photoemission spectroscopy (XPS), near edge X-ray absorption

fine structure (NEXAFS) spectroscopy, and atomic force microscopy (AFM) on nanorods deposited on Au(111) and Au(110) single crystals. XPS thickness dependent spectra in combination with NEXAFS investigations show that the screening of the core hole occurs via charge transfer from the metal to the molecule. In addition, the morphology of the nanorods has been investigated by using AFM, evaluating the nanorod characteristics also from a statistical point of view and taking the different degree of fluorination into account.

CPP 29.9 Wed 18:00 H33

Photoemission Investigation of the Electronic Structure of P3HT:PCBM Bulk-Heterojunctions using a lift-off technique — ●ANGELA ECKSTEIN^{1,2}, DIRK HAUSCHILD^{1,2}, JULIA KERN³, MARKUS MINGEBACH³, CARSTEN DEIBEL³, VLADIMIR DYAKONOV³, ACHIM SCHÖLL^{1,2}, and FRIEDRICH REINERT^{1,2} — ¹Experimentelle Physik VII, Universität Würzburg, 97074 Würzburg — ²Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, 76021 Karlsruhe — ³Experimentelle Physik VI, Universität Würzburg, 97074 Würzburg

Poly(3-hexylthiophene): phenyl-[6,6]-C61 butyric acid methyl ester (P3HT:PCBM) bulk heterojunctions (BHJ) are prototype active layers for organic solar cells. The electronic structure at the internal interface can be accessed by photoelectron spectroscopy (PES), thus providing insight into the alignment of the electronic levels and the occurrence of possible interface dipoles. However, the very surface sensitive PES investigation is complicated in case of P3HT:PCBM bulk heterojunctions since the film preparation by spin-coating creates a P3HT wetting layer on the film surface. In order to avoid this problem we used a lift-off technique to access the interface to the spin coating substrate (SiO₂), which has shown to resemble the bulk situation [1]. P3HT:PCBM samples with different mixing ratio, which can be lift-off-prepared under UHV-condition thus avoiding contamination by ambient conditions, have been investigated by x-ray- and UV-PES as well as by inverse PES with particular respect to the influence of degradation and radiation damage. [1] Kahn et al. (*Org. El.* 11 (2010) 1779-1785)

CPP 29.10 Wed 18:15 H33

Bottom-up synthesis of self-aligned conjugated polymers — SÖREN KROTZKY¹, ●RICO GUTZLER¹, VIJAY VYAS^{1,2}, BETTINA LOTSCH^{1,2}, and KLAUS KERN^{1,3} — ¹Max Planck Institute for Solid State Research, Stuttgart, Germany — ²Department of Chemistry, University of Munich (LMU), Munich, Germany — ³Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, Switzerland

We investigate the synthesis of self-assembled organometallic structures and well-defined long 1D polymers by the surface-supported Ullmann reaction on an Ag(111) surface. The brominated semiconducting precursor molecule (2,7-dibromobenzothieno[3,2-b]benzothiophene) is sublimed under UHV conditions on the crystalline surface where a dehalogenation step is induced at room temperature. STM reveals self-assembly of the dehalogenated ditopic molecule into short organometallic coordination polymers that arrange in a ladder-like monolayer. Annealing to 420 K leads to C-C coupling of the molecules via ejection of the coordinated metal atom. At this temperature the newly formed 1D polymer strands align in a side-by-side manner with three preferred directions with respect to the high-symmetry directions of the surface. DFT calculations show that the length of the synthesized polymers is sufficient to reduce the HOMO-LUMO gap to its value at infinite length of the polymer. Together with the calculated band-structure this suggests possible unidirectional charge mobility within the well-ordered semiconducting polymeric monolayer.

CPP 29.11 Wed 18:30 H33

How contact groups influence metal molecule hybrid structures under voltage — ●SIMON LIEBING, TORSTEN HAHN, and JENS KORTUS — TU Bergakademie Freiberg, Freiberg, Germany

In order to use molecules in electronics it is not only important to understand the properties of molecules themselves but also properties of metal-molecule interfaces. Recent contributions discussed the behavior of thiole [1] and amino linker groups [2]. To get a more systematic understanding the authors have chosen a model system of benzene with variable linker groups between gold electrodes. Such groups can be thiole, amino, thiophen, nitrile, pyrrol and cyanide. This allows for example to study the differences between σ - and π -like symmetry with respect to the individual interface geometry. The theoretical study combines the calculation of single molecule properties by density

functional theory [3] with the nonequilibrium Greens functions technique [4] to calculate the transport properties [5] of the device. [1] Markussen, T. et al. JCP **132**, 224104 (2010)

[2] Angela, D. et. al. Nano Letters **10**, no. 7 (2010)

[3] Pederson, M. et. al. Phys. Status Solidi b **217**, 197. (2000)

[4] Datta, S. Nanotechnology **15**, 433. (2004)

[5] Brandbyge, M. Phys. Rev. B **65**, 165401 (2002)

CPP 29.12 Wed 18:45 H33

Improving the contact materials of organic electronic devices: Polymeric dipole layers vs. self assembling monolayers — ●JANUSZ SCHINKE^{1,2}, JULIAN HEUSSER^{3,2}, MARC HÄNSEL^{3,2}, JULIA MAIBACH^{4,2}, WOLFGANG KOWALSKY^{1,2}, MICHAEL KRÖGER^{1,2}, ERIC MANKEL^{4,2}, and WOLFRAM JAEGERMANN^{4,2} — ¹TU Braunschweig, Institut für Hochfrequenztechnik — ²Innovation Lab GmbH — ³Universität Heidelberg, Kirchhoff-Institut für Physik — ⁴TU Darmstadt, Materials Science Institute, Surface Science Division

In organic electronic devices, charge injection at the contacts is crucial for high electrical performance. Most of these devices require at least one electrode with a sufficiently low work function (WF). Low-WF electrodes like alkaline earth metals are easily available; however, they are chemically very reactive and oxidize in ambient atmosphere. A smart way to overcome this problem is the use of molecular or polymeric dipole layers (PDLs). The use of PDLs to tune an electrodes work function can be advantageous over self assembled monolayers(SAMs) as the PDL concept can be applied to a wider range of electrode materials like ITO, Ag, Au or Al. We have used two different PDLs: branched polyethylenimine (PEI) and polyethylenimine ethoxylate (PEIE). We studied the the properties of PDL treated substrates via AFM, ambient Kelvin probe and XPS/UPS. Both interlayers lower the metal substrate work function by approx. 1000meV. On ITO we reach absolute values of about 3.0eV which leads to strongly enhanced electron injection in model devices.

CPP 30: Poster: Focus: Wetting on smooth and rough surfaces: From spreading to superhydrophobicity

Time: Wednesday 16:30–18:30

Location: Poster C

CPP 30.1 Wed 16:30 Poster C

Polymer brushes in poor solvent - A Monte Carlo Study — ●CHRISTOPH JENTZSCH^{1,2} and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden, Germany — ²TU-Dresden, Institut für theoretische Physik, Germany

We use a new variant of the bond fluctuation model with explicit solvent to study polymer brushes under poor solvent conditions. Extensive simulations were performed in order to cover a wide range of grafting densities for large systems. For high grafting densities we observe a dense uniform brush. By decreasing the grafting density, we observe stable holes penetrating through the brush. A further decrease of the grafting density leads to a semicontinuous morphology due to a segregation between the solvent and the polymers. For very low grafting densities we observe octopus micelles of different sizes. We investigate those regimes and their transitions.

CPP 30.2 Wed 16:30 Poster C

Droplet morphologies upon growing and shrinking on triangular grooved substrates — ●CARSTEN HERRMANN¹, CIRO SEMPREBON², MARTIN BRINKMANN^{1,2}, and RALF SEEMANN¹ — ¹Saarland University, 66041 Saarbrücken — ²Max Planck Institute for Dynamics and Self-Organization, 37018 Göttingen

We experimentally investigate the morphologies of droplets sitting on triangular grooved micro-structures upon volume change. The droplet morphologies are characterized by their eccentricity, i.e. the ratio of width to length, as function of the number of wetted grooves. The eccentricity of small droplets wetting just a few grooves characteristically varies upon an increase in drop volume and arrives at a constant value for sufficiently large droplets. In contrast droplets are almost perfectly round upon volume reduction for sufficiently small droplet volumes. In both cases the morphological changes depend sensitively on the wettability and the wedge angle of the triangular grooved substrate. The experimental results are compared quantitatively with numerical results computed by minimizing surface energies.

CPP 30.3 Wed 16:30 Poster C

Liquid-liquid dewetting — ●STEFAN BOMMER¹, SEBASTIAN JACHALSKI², DIRK PESCHKA², RALF SEEMANN¹, and BARBARA WAGNER² — ¹Saarland University, 66041 Saarbrücken — ²Weierstraß-Institute, 10117 Berlin

The transient morphologies towards equilibrium of liquid droplets dewetting on another liquid are considered experimentally and theoretically. As liquids short chained polystyrene and polymethylmethacrylate are used which are glassy at room temperature and which can be considered as Newtonian liquids well above their glass transition temperatures. The liquid/air interfaces are imaged in situ by scanning force microscopy whereas the liquid/liquid interface is imaged after solidifying the sample and removing the dewetting polystyrene. The obtained droplet shapes are compared to numerical results in lubrication approximation which are calculated for the surface tensions and contact angles which are extracted from the equilibrium shapes of

the droplets. A remarkable independence of the transient shapes on the start conditions was found for sufficiently 'mature' droplets which allows for the quantitative comparison.

CPP 30.4 Wed 16:30 Poster C

Light induced switching of surface wetting of azobenzene decorated silicon nanograss surfaces — ●JONAS GROTEN and JÜRGEN RÜHE — Universität Freiburg, IMTEK

The wetting behavior of high aspect ratio nanorough surfaces depends on the surface energy of the involved materials. Depending on the value of the surface energy superwetting, Wenzel type wetting or superhydrophobicity can be observed. These wetting regimes are separated by sharp transitions at well defined surface energies. We have coated a silicon surface consisting of high aspect ratio nanoscale needles ("black silicon") with a polymer monolayer containing a fluorinated azobenzene moiety. The azobenzene moiety can be switched between the cis and the trans state through illumination with light of appropriate wavelengths. In the described system the surface energy of the polymer coating is adjusted to the energy value which separates the distinct wetting regimes of the nanorough surface. This coupling allows for large changes in the surface wetting behavior even when the surface energy upon illumination is only rather small. As a consequence the surface can be reversibly switched from a superhydrophobic state with roll off tilt angle $< 2^\circ$ to a completely sticky surface with no roll off at all or from a strong Wenzel-type wetting state to a superwetting surface.

CPP 30.5 Wed 16:30 Poster C

Transformation of black candle soot into a transparent robust superamphiphobic coating — ●XU DENG, LENA MAMMEN, PERIKLIS PAPADOPOULOS, MAXIME PAVEN, HANS-JÜRGEN BUTT, and DORIS VOLLMER — Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany

Coating is an essential step in adjusting the surface properties of materials. Superhydrophobic coatings with contact angles greater than 150° and roll off angles below 10° for water have been developed, based on low energy surfaces and roughness on the nano- and micrometer scales. However, these surfaces are still wetted by organic liquids such as surfactant-based solutions, alcohols, or alkanes. Coatings that are simultaneously superhydrophobic and superoleophobic are rare. We designed an easily fabricated, transparent, and oil-rebounding superamphiphobic coating. A porous deposit of candle soot was coated with a 25 nm thick silica shell. The black coating became transparent after calcination at 600°C . After silanization the coating is superamphiphobic and remained so even after its top layer was damaged by sand impingement.

CPP 30.6 Wed 16:30 Poster C

The Salvinia Effect: Superhydrophobic Surfaces with Hydrophilic Pins for Air Retention Under Water — ●DANIEL GANDYRA¹, BIRTE BÖHNLEIN¹, MATTHIAS MAIL^{1,2}, AARON

KOBLER¹, ANKE KALTENMEIER¹, MATTHIAS BARCZEWSKI¹, STEFAN WALHEIM¹, KERSTIN KOCH⁴, JAN-ERIK MELSKOTTE³, MARTIN BREDE³, ALFRED LEDER³, WILHELM BARTHOLOTT², and THOMAS SCHIMMEL¹ — ¹Institute of Applied Physics, Institute of Nanotechnology, and Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology — ²Nees Institute for Biodiversity of Plants, University of Bonn — ³Chair of Fluid Mechanics, University of Rostock — ⁴Biology and Nanobiology, Hochschule Rhein-Waal

Air-retaining surfaces are of great technological, economic and ecological interest, e.g., for low-friction fluid transport and drag reduction in ship coatings. An innovative mechanism for long-term air retention under water is found in the sophisticated surface design of water fern *Salvinia molesta*. Its floating leaves are evenly covered with complex hydrophobic hairs retaining a layer of air when submerged under water. The terminal cells of the hairs, however, are hydrophilic. These hydrophilic patches at the end of the hairs pin the air-water interface, thus preventing the loss of air by preventing the formation and detachment of air bubbles [1]. This "Salvinia Effect" opens intriguing perspectives for developing artificial, biomimetic surfaces with long-term air retention under water. [1] W. Barthlott, T. Schimmel et al.: The Salvinia Paradox. *Advanced Materials* 22, 2325-2328, 2010.

CPP 30.7 Wed 16:30 Poster C

Drop impact on superamphiphobic surfaces — ●XU DENG¹, FRANK SCHELLENBERG¹, PERIKLIS PAPADOPOULOS¹, LONGQUAN CHEN², MAXIME PAVEN¹, LENA MAMMEN¹, JIHUA ZHANG¹, DORIS VOLLMER¹, and HANS-JÜRGEN BUTT¹ — ¹Max Planck Institute for Polymer Research, Mainz — ²Center of Smart Interfaces, Technical University Darmstadt

The spreading and retraction kinetics of liquid drops impacting on superamphiphobic,[1] i.e. superhydrophobic and superoleophobic, surfaces is studied by high speed video microscopy. To investigate the influence of interfacial tension and viscosity on spreading and retraction kinetics mixtures of ethanol-water and glycerin-water are chosen. The main findings are identical for both systems, including the dependence of the impact scenario on drops' Weber and Reynolds number. At low impact velocity the drops rebound, however, the contact time increases when approaching the pinning regime. Drop spreading is dominated by inertia, independent of whether a drop rebounds or pins on the surface. The retraction phase is split into two regimes: a fast inertia dominated retraction of the drop's contour, followed by a slow decrease of the drop's contact diameter for diameters below the initial diameter of the drop before impact. Impact causes partial penetration and pinning of the liquid in the coating, even though the drop rebounds completely.

[1] X. Deng, L. Mammen, H.-J. Butt, and D. Vollmer; *Candle soot as a template for a transparent robust superamphiphobic coating*, *Science*, 335 (2012), 67-70.

CPP 30.8 Wed 16:30 Poster C

Simulating immiscible multi-phase flow and wetting by means of stochastic rotation dynamics (SRD) - A 3D modeling approach — ●THOMAS HILLER, MARTA SANCHEZ DE LA LAMA, MARTIN BRINKMANN, and STEPHAN HERMINGHAUS — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

We use the mesoscopic particle simulation method SRD to simulate immiscible multi-phase flow on the pore and sub-pore scale in three dimensions. As an extension to the standard SRD method, we present a novel approach on implementing complex wettability on heterogeneous surfaces. Our preliminary results demonstrate the capability of this method to address a variety of applications. For instance, on the pore-scale SRD is a valuable tool to study the formation of capillary bridges in an assembly of three or four spherical beads. Additionally, we show the simulation of flow through an artificial porous media (packing of spherical beads) where the substrate exhibits different spatial wetting characteristics and how this influences the dynamics, in terms of percolation and residual saturation, through the porous media. As an outlook we also present how SRD can be applied to simulate droplets flowing in microfluidic channels.

CPP 30.9 Wed 16:30 Poster C

Transparent silica nano- and microchannels for microfluidic devices — ●LENA MAMMEN, XU DENG, KATHRIN FRIEDEMANN, FRANK SCHELLENBERGER, PERIKLIS PAPADOPOULOS, DANIEL CRESPY, HANS-JÜRGEN BUTT, and DORIS VOLLMER — Max Planck Institute for Polymer Research, Mainz, Germany

Nano- and microchannels are attractive model systems for fundamental studies like filling kinetics, diffusion processes or transport phenomena. In this work transparent nano- and few-micrometer-sized silica channels were prepared by coating different polymer fiber templates with silica performing a modified Stöber synthesis and subsequent removal of the organic material by calcination. As templates either PVA or polystyrene electrospun or spider silk fibers were used. The channels have a circular cross-section with uniform diameter and smooth surface. We measured the capillary filling speed of water and glycerol/water mixtures and castor oil using laser scanning confocal microscopy (LSCM) what is a convenient technique to observe the filling velocities close to the channel entrance. By comparing our results with the theoretically predicted values according to the classical Washburn kinetics we found a deviation for small filling times (< 0.1 s) from the power law.

CPP 30.10 Wed 16:30 Poster C

Microcones and Nanograss: Towards mechanically robust superhydrophobic surfaces — ●VITALIY KONDRASHOV and JÜRGEN RÜHE — University of Freiburg, Freiburg, Germany

We report on the generation of superhydrophobic surfaces, which are resistant to strong mechanical forces, especially against high shear stress. To this we generate surfaces, which have two roughness levels: micrometer sized silicon microcones surrounded by superhydrophobic silicon nanograss. The fabrication process of the surface is mask-free, and both microcones and nanograss are fabricated in consecutive processes by Deep Reactive Ion Etching (DRIE) in the overpassivation regime. Varying the process parameters, microcones of different size and density were fabricated, while nanograss size and distribution were kept constant.

When shear is applied, the microcones take the load and prevent contact of the shearing surface with the mechanically instable silicon nanograss. As the microcones can cause pinning of the contact line, the height and density of the microcones are important parameters for the influence of wear onto the wetting properties. As result, the shear-stress experiments show that surfaces with high density of large microcones are able to sustain high shear loads without noticeable loss in superhydrophobicity. However, the larger the microstructures the larger shaved hydrophilic area which increases pinning to the drop. This shows that, the control over microcones size and density is a key factor in realization of mechanically robust superhydrophobic surfaces.

CPP 30.11 Wed 16:30 Poster C

Influence of subsurface interactions on the dynamic contact angle of liquids on mixed organic monolayers — DAVID POLSTER¹ and ●HARALD GRAAF² — ¹Department of Physics, University of Konstanz, D-78464 Konstanz, Germany — ²nanoMA (Center for nanostructured Materials and Analytics), Chemnitz University of Technology, D-09107 Chemnitz, Germany

The functionalisation of surfaces by organic monolayers is a well known way to influence the surface properties e.g. the adhesion forces. Mixed monolayers consisting of similar molecules with two or more various headgroups can tune the obtained surface properties like the hydrophobicity. In the present study silicon surfaces are modified by alkene molecules. By using two different alkenes mixed monolayers of various ratios the hydrophilicity of the surface can be tuned. A water ring formation around single and double ester groups increase the effective hydrophilic area, which leads to a deviation from the expected change in static contact angle measurements.[1] In a recent study we found on such mixed monolayers a hysteresis of the dynamic contact angle of different liquids.[2] Several approaches are discussed in literature the hysteresis (and also differences in wetting and dewetting energies) partially to long range interactions between the liquid and the underlying silicon, which is very reasonable as the monolayer thickness is only about two nanometers.

[1] Polster et al. *Langmuir* 26 (2010) 8301, [2] Polster et al. *Appl.Surf.Sci.* DOI 10.1016/j.apsusc.2012.10.128

CPP 30.12 Wed 16:30 Poster C

Universal Phase Diagram for Wetting on Mesoscale Roughness — ●STEPHAN HERMINGHAUS — MPI für Dynamik und Selbstorganisation

The wetting properties of solid substrates with mesoscale (between van der Waals tails and the capillary length) random roughness are considered as a function of the microscopic contact angle of the wetting liquid and its partial pressure in the surrounding gas phase. It is shown that the well-known transition occurring at Wenzel's angle is accom-

panied by a transition line at which a jump in the adsorbed liquid volume occurs. This should be present generally on surfaces bearing homogeneous, isotropic random roughness. While a similar abrupt filling transition has been reported before for certain idealized groove or trough geometries, it is identified here as a universal phenomenon. Its location can be analytically calculated under certain (rather mild) conditions.

CPP 30.13 Wed 16:30 Poster C

Patterning of YVO₄:Eu³⁺ luminescent films by soft lithography — ●WENXIN WANG¹, ZIYONG CHENG², JUN LIN², and YONG LEI¹ — ¹Fachgebiet 3D-Nanostrukturierung, Institut fuer Physik & IMN MacroNano (ZIK), Institute for Physics and IMN MacroNano (ZIK), Technische Universitaet Ilmenau, Prof. Schmidt Str. 26, 98693 Ilmenau, Germany — ²State Key Laboratory of Rare Earth Resource Utilization, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, 5625 Renmin Street, Changchun 130022, P.R.China

Ordered square and dot luminescent YVO₄:Eu³⁺ array patterns were fabricated by two kinds of soft lithography processes, namely, microtransfer molding (uTM) and microcontact printing (uCP), respectively. Both soft-lithography processes utilize a PDMS elastomeric mold as the stamp combined with a Pechini-type sol-gel process to produce luminescent patterns on quartz plates. The difference is that square pattern can be direct obtained via uTM, but with method of uCP, we print hydrophobic SAMS on the hydrophilic quartz to induce the dewetting process of sol precursor to form dot pattern array.

The ordered luminescent YVO₄:Eu³⁺ patterns are revealed by optical microscopy and their microstructures, consisting of nanometer-scale particles, is unveiled by scanning electronic microscopy (SEM) observations. Additionally, photoluminescence and cathodoluminescence were carried out to characterize the patterned YVO₄:Eu³⁺ samples.

CPP 30.14 Wed 16:30 Poster C

Wetting of silica spheres on the micro-scale — ●JENNIFER WENZL, RENÉ STANGENBERG, and GÜNTER K. AUERNHAMMER — Max Planck Institute for Polymer Research, Mainz, Germany

We present here a model system for wet granular matter on the micrometer scale, which we are able to observe in 3D with confocal microscopy. We use a 3-phase-system consisting of polydisperse silica particles, dispersed in a mixture of an aqueous salt solution (sodium thiocyanate) and an organic solvent (cis-decaline). By mere shaking of the sample mixture, we generate capillary bridges and pickering emulsion droplets with cis-decaline as the binder liquid. Surface modification with methyl silyl groups allows us to adjust a finite contact angle of the interface between the binder liquid and the aqueous salt solution. With the combination of the confocal microscopy and a home-build nano-manipulation, we are able to apply a compression or shear load and observe simultaneously the sample structure in 3D.

We investigated the particle-droplet structure in 3D under compression and shear. In this presentation we show the wetting behavior of this interface and discuss the change of the emulsion droplet number and the corresponding volumes with time. We present also the structural changes of the particles depending on the applied load.

CPP 31: Poster: Organic Electronics and Photovoltaics (joint session DS/HL/O/CPP)

Time: Wednesday 16:30–18:30

Location: Poster C

CPP 31.1 Wed 16:30 Poster C

Templating effects of 6T layers for organic DIP layers — ●CHRISTOPHER LORCH, ALEXANDER HINDERHOFER, RUPAK BANERJEE, CHRISTIAN FRANK, JOHANNES DIETERLE, ALEXANDER GERLACH, and FRANK SCHREIBER — Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Recently, the donor-acceptor combination of the two compounds, α -sexithiophene (6T) [1] and diindenoperylene (DIP) [2], respectively, has shown an extraordinarily high open circuit voltage in organic solar cells with a planar heterojunction (PHJ) architecture [3].

Synchrotron based real-time *in situ* X-ray diffraction experiments were performed to study the temperature-dependent growth characteristics of 6T. Furthermore, the influence of the structural properties of the 6T layer on the top DIP layer were investigated. In this contribution, the following points are discussed: i) Dependence of the ratio of lying and standing domains in the top DIP layer on the corresponding ratio in the bottom 6T layer. ii) The thickness dependence of the DIP layer structure. iii) Possible reorganization effects in the bottom layer during the growth of the top layer. iv) The dependence of top layer structure on the temperature.

[1] W. Steinkopf *et al.*, Justus Liebig's Ann. Chem. 546, 180-199 (1941)

[2] A. C. Dürr *et al.*, Phys. Rev. Lett. 90, 016104 (2003)

[3] U. Hörmann *et al.*, Phys. Status Solidi RRL 5, 241-243 (2011)

CPP 31.2 Wed 16:30 Poster C

Solution processed of self-assembled monolayers as charge injection layers in organic FETs. — ●MILAN ALT^{1,4}, JANUSZ SCHINKE^{2,4}, KAJA DEING^{3,4}, ULI LEMMER¹, and NORMAN MECHAU^{1,4} — ¹Karlsruher Institute of Technology — ²TU Braunschweig — ³Merck KGaA, Darmstadt — ⁴InnovationLab, Heidelberg

All-solution processed organic field effect transistors (OFETs) are expected to play a key role in the mass production of organic electronic devices via high throughput printing techniques. In this study we focus on solution processing of self-assembled monolayers (SAMs) for enhancement of charge carrier injection at the metal-semiconductor interface. One necessity in order to make SAMs printable is an understanding of molecular assembly in dependency to process parameters like accumulation time and molecular concentration in the solution. We used well established benchmark materials to investigate the functionality of different benzyl-mercaptan and alkanethiol SAMs in OFETs. The methodic evaluation of OFET devices, in which the transistor effectively serves as a characterization tool, revealed an expected corre-

lation between metal work function shift and device threshold voltage. More interestingly, an optimum ratio of accumulation time/SAM concentration has been identified. In contrast, investigations of SAM isle accumulation on crystalline Au 111 surfaces in literature reveal a saturation of work function shift when approaching a closed monolayer. This demonstrates that understanding of SAM growth mechanisms gained on single crystalline surfaces cannot naturally be transferred to assembly on printed or evaporated metal contacts.

CPP 31.3 Wed 16:30 Poster C

Photophysical Processes in Polymer:PDI Solar Cells — ●DOMINIK GEHRIG, VALENTIN KAMM, HANNAH MANGOLD, IAN HOWARD, GLAUCO BATTAGLIARIN, CHEN LI, KLAUS MÜLLEN, and FRÉDÉRIC LAQUAI — Max-Planck-Institute for Polymer Research, Mainz, Germany

We present the implementation of different polymers as donors in combination with new PDI-based acceptors in organic solar cells. Increasing the absorption of the photoactive layer is a rational strategy that could give rise to an enhanced photon harvesting and hence an improvement of the photocurrent. The contribution of PDI to the photocurrent generation can be proved by EQE measurements. Additionally exciton and charge carrier dynamics as well as loss mechanisms are investigated by sub-picosecond to millisecond pump-probe transient absorption spectroscopy (TA) and time-resolved photoluminescence (TRPL) spectroscopy. The former tracks the dynamics of non-radiative species whereas the latter enables the observation of emissive decay channels. Supplementary experiments like the evaluation of the morphology by AFM and charge transport experiments by the time-of-flight (TOF) technique and space-charge-limited-current (SCLC) measurements deliver additional information which allow to derive meaningful structure-property-relations.

CPP 31.4 Wed 16:30 Poster C

Increased conductivity of PEDOT:PSS for application in organic solar cells: electrical and morphological investigations — ●CHRISTOPH HELLER¹, CLAUDIA M. PALUMBINY¹, VOLKER KÖRSTGENS¹, YUAN YAO¹, WEIJIA WANG¹, STEPHAN V. ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Frank-Str. 1, 85748 Garching, Germany — ²HASYLAB at DESY, Notkestrasse 85, 22603 Hamburg, Germany

Poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate)(PEDOT:PSS) is commonly used as a transparent electrode for flexible electronic de-

vices. Its conductivity plays a crucial role for the device performance.

In our study, the conductivity of PEDOT:PSS films has been increased via a post treatment method reaching the conductivity order of indium tin oxide (ITO) which is commonly used as an electrode in organic solar cells. Among other techniques the effect of the post treatment has been investigated using advanced scattering methods such as grazing incident small angle x-ray scattering (GISAXS). Furthermore, the influence of doping PEDOT:PSS, different post treatments, the treatment time and the effect of the number of post treatments have been investigated focusing on conductivity and morphological changes. The results are very promising for using post treated PEDOT:PSS as an electrode in ITO-free organic solar cells.

CPP 31.5 Wed 16:30 Poster C

Low-bandgap DPP-type Polymers for OPVs: Relation between Device Performance and Photophysical Properties — ●JULIAN OCHSMANN¹, MATHIEU TURBIEZ², DEEPAK CHANDRAN³, IAN HOWARD¹, KWANG-SUP LEE³, and FRÉDÉRIC LAQUAI¹ — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²BASF, Basel, Switzerland — ³Hannam University, Seoul, Korea

Low-bandgap polymers are promising materials to serve as electron donors in the photoactive layer of bulk heterojunction solar cells. In combination with a suitable electron acceptor such as PC70BM the photoactive layer covers a broad absorption range spanning from the visible to the near-infrared spectral region leading to increased photon harvesting and thus a higher photocurrent compared to mid-bandgap polymers such as P3HT.

In this study the photovoltaic performance of several low-bandgap polymers based on the diketopyrrolopyrrole (DPP) unit was evaluated in Organic Photovoltaic Cells (OPVs) prepared with different solvent mixtures. Depending on the polymer structure and preparation conditions maximum power conversion efficiencies between 1.6 and 5 % could be reached. The photophysical properties of the photoactive layers of the OPVs were investigated by steady-state photoinduced absorption and broadband transient absorption pump-probe spectroscopy (TA) to get further insight into the exciton and polaron dynamics as well as into the efficiency-limiting mechanisms of the devices.

CPP 31.6 Wed 16:30 Poster C

Investigation of Polyethylenimine and Polyethylenimine-ethoxylated as electron injection layers in solution processed organic light-emitting diodes. — ●SEBASTIAN STOLZ^{1,4}, INGO RINGLE², ERIC MANKEL^{3,4}, JANUSZ SCHINKE⁴, MICHAELA AGARI², GERARDO HERNANDEZ-SOSA^{1,4}, WOLFRAM JAEGERMANN^{3,4}, ULI LEMMER¹, and NORMAN MECHAU^{1,4} — ¹Light Technology Institute, Karlsruhe Institute of Technology — ²Pre-development, Heidelberger Druckmaschinen AG — ³Materials Science Institute, Technische Universität Darmstadt — ⁴InnovationLab GmbH, Heidelberg

One obstacle for inexpensive solution processed organic light-emitting diodes (OLEDs) is the current use of low work-function metals like calcium or barium as cathode materials. These metals are highly reactive, which is why they cannot be easily solution processed but have to be prepared in UHV. In this work, we investigate two organic polymers, Polyethylenimine (PEI) and Polyethylenimine-ethoxylated (PEIE), which are known to reduce the work-function of various metals, for their applicability as electron injection layers. Therefore, both polymers are dissolved in 2-Methoxyethanol with varying concentrations and are then spin coated on top of Aluminum substrates. The concentration dependent change in work-function is determined by kelvin probe measurements and ultraviolet photoemission spectroscopy. Furthermore, OLEDs using PEI, or PEIE respectively, as electron injection layer are prepared by spin coating. Compared to reference devices with calcium as electron injection material, these OLEDs show comparable turn on voltages and luminance values of more than 50%.

CPP 31.7 Wed 16:30 Poster C

Surface morphology of P3HT, PCBM and blends of both — ●MARTIN DEHNERT¹, MARIO ZERSON¹, SVEN HÜTTNER², ZHUXIA RONG², ULLRICH STEINER², and ROBERT MAGERLE¹ — ¹Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Chemnitz, Germany — ²Cavendish Laboratory, JJ Thomson Avenue, Cambridge, U.K.

We investigate the surface morphology of thin films of pure poly(3-hexylthiophene) (P3HT), [6,6]-phenyl C61-butyric acid methyl ester (PCBM) and blends of P3HT and PCBM using atomic force microscopy (AFM) operated in multi-set point intermittent contact (MU-

SIC) mode. This allows for depth-resolved mapping of the mechanical properties of the top surface layer of the specimen. AFM images of pure P3HT and PCBM before and after annealing show the crystallization behaviour of the pure materials at the film surface. Blends of P3HT and PCBM with different composition were used for investigating the morphology, the nanomechanical properties, and the composition of the top surface layer. Our results indicate that for large range of blend compositions the volume ratio of P3HT and PCBM is constant within the top surface layer. Furthermore, we observe crystallisation of PCBM in films annealed at 175°C. We discuss the impact of the surface morphology of P3HT:PCBM blends and the crystallisation of PCBM on the efficiency and lifetime of organic solar cells.

CPP 31.8 Wed 16:30 Poster C

Probing charge carrier dynamics in organic solar cells based on merocyanines — ●STEVEN GRAF¹, MARTIN LENZE¹, JULIAN KRUMRAIN¹, DIRK HERTEL¹, KLAUS MEERHOLZ¹, and FRANK WÜRTHNER² — ¹Department für Chemie, Universität zu Köln, Luxemburger Straße 116, 50939 Köln — ²Institut für Organische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg

Organic photovoltaics offer a very promising green energy alternative. Highly efficient organic solar cells can be produced by cost-effective methods such as coating from solution (SOL) or depositing under high vacuum conditions (VAC). In our approach we investigate merocyanines (MC), a class of low-molecular-weight colorants, as donor material in organic BHJ solar cells. These molecules are processable via both deposition techniques showing remarkable power conversion efficiencies (PCE) beyond 4% for SOL- and 6% for VAC-processed devices. Towards even higher PCEs it is mandatory to obtain a better insight into fundamental charge carrier processes such as generation, transport and recombination. We use steady state and time resolved photoluminescence spectroscopy to examine charge-transfer (CT) states in pure and blended merocyanine thin films. The role of these CT states in solar cells is further studied by field and temperature dependent measurements of the external quantum efficiency (EQE). By varying processing conditions as well as blend compositions the influence of morphology on the solar cells is illustrated. The investigations are supported by temperature and electric field dependent studies of charge recombination and transport via photo-CELIV technique.

CPP 31.9 Wed 16:30 Poster C

Influence of different alkyl side chains on merocyanine dye performance in organic solar cells — ●JULIAN KRUMRAIN¹, ALHAMA ARJONA ESTEBAN², STEVEN GRAF¹, MARTIN LENZE¹, DIRK HERTEL¹, FRANK WÜRTHNER², and KLAUS MEERHOLZ¹ — ¹Department für Chemie, Universität zu Köln, Luxemburger Straße 116, 50939 Köln (Germany) — ²Institut für Organische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg (Germany)

In recent years, organic photovoltaics have attracted great attention as an alternative energy source due to their reduced cost and easier processability, compared to inorganic materials. Specifically, small-molecule dyes have achieved great strides in recent years reaching power conversion efficiencies up to 7%. These dyes have advantages over polymers, most notably their simplified, large-scale syntheses and purification. Furthermore small molecules can be processed either by solution or vapor-deposition processes. We have investigated organic solar cells based on merocyanine (MC) dyes as an electron donor material in vacuum-deposition processed bulk-heterojunctions (BHJ). In order to get a better understanding of the influence of side chains on the MC dyes in BHJ, we have synthesized MC dyes with different alkyl side chain lengths. We have carried out temperature and light intensity dependent current-voltage measurements as well as atomic force microscopy studies. It becomes apparent that the BHJ morphology is strongly influenced by the side chain length. The short-circuit current density decreases enormously for increasing side chain length in complete contrast to the solubility of the MC dyes.

CPP 31.10 Wed 16:30 Poster C

Absorption and exciton management in DIP/C₆₀ bilayer photovoltaic cells — ●A. STEINDAMM^{1,2}, M. BRENDEL^{1,2}, K. TOPCZAK¹, and J. PFLAUM^{1,2} — ¹Exp. Phys. VI, University of Würzburg, 97074 Würzburg — ²ZAE Bayern, 97074 Würzburg

The combination of the promising material Diindenoperylene (DIP) with the acceptor C₆₀ has led to overall efficiencies up to 4 % in organic photovoltaic cells (OPVCs) [1]. A drawback in performance is found in the rather poor light absorption of the crystalline DIP layer due to its unfavorable orientation of transition dipoles perpendicular

to the electric field vector of incident light. Therefore we pursued different approaches for increasing the current density. First, the orientation of the individual DIP molecules was altered by varying the growth conditions in order to increase light absorption. Second, the interface effects of an Bathophenanthroline (BPhen) exciton blocking layer (EBL) on the exciton management in DIP/C₆₀ were investigated by a complementary study of current density, external quantum efficiency, and photoluminescence quenching for various EBL thicknesses. These investigations reveal exciton losses by contact metal quenching in both active layers if no EBL is applied. In contrast, an optimal trade-off between exciton blocking, suppression of metal penetration, and electron transport is achieved for a 5 nm thick BPhen layer yielding an improvement of power conversion efficiency by more than a factor of 2 [2]. Financial support by BMBF (GREKOS) and DFG (SPP1355) is acknowledged.

[1] A. Opitz, et al., IEEE J. Sel. Top. Quant. El. 16, 1707 (2010)

[2] A. Steindamm, et al., Appl. Phys. Lett. 101, 143302 (2012)

CPP 31.11 Wed 16:30 Poster C

The effect of fluorination on the performance of F_nZnPc/C₆₀ organic photovoltaic cells — ●M. BRENDL^{1,2}, A. STEINDAMM^{1,2}, F. STAUB¹, and J. PFLAUM^{1,2} — ¹Exp. Phys. VI, University of Würzburg, 97074 Würzburg — ²ZAE Bayern, 97074 Würzburg

The material class of phthalocyanines has proven to be a suited donor material in small molecule organic photovoltaic cells (OPVCs). Planar heterojunctions based on zinc phthalocyanine (ZnPc) in combination with the acceptor C₆₀ show high short circuit currents (*j_{sc}*) of 6.3 mA/cm² and fill factors (FF) of 51 % [1]. However, due to the small effective band gap *E_{g,eff}* of only 1 eV between ionisation potential of the donor and electron affinity of the acceptor, the correlated open circuit voltage (*V_{oc}*) is limited to 0.5 V. As a possible approach energy levels of Pcs can be modified by substituting hydrogen atoms. With increasing degree of fluorination the position of the HOMO and LUMO levels are shifted to lower energies. In this contribution we investigated the impact of *E_{g,eff}* on *V_{oc}* for a varying degree of fluorination (*n* = 0, 4, 8, 16) in F_{*n*}ZnPc/C₆₀ OPVCs. First results revealed a significant *V_{oc}* improvement of 20 % to 0.6 V for F₄ZnPc based cells compared to ZnPc, while *j_{sc}* and FF ideally remained unaffected. However, the gain in *V_{oc}* is smaller than expected by the difference in ionisation potential which accounts for 0.2 - 0.4 eV. This discrepancy will be analyzed in our studies and will lead to a deeper insight into the origins of *V_{oc}* and its correlation to the energetics on the molecular entities. Financial support by the BMBF (project GREKOS) and by the DFG (program SPP1355). [1] Z. R. Hong, et al., Appl. Phys. Lett. 2007, 90, 203505

CPP 31.12 Wed 16:30 Poster C

Surface Structure of organic solar cells based on PBDTTT-C and PC70BM — ●MARIO ZERSON¹, ANDREAS ZUSAN², CARSTEN DEIBEL², and ROBERT MAGERLE¹ — ¹Chemische Physik, Technische Universität Chemnitz, Chemnitz, Germany — ²Experimental Physics VI, Julius-Maximilians-University of Würzburg, Würzburg, Germany

We study the surface structure of organic heterojunction solar cells based on blends of poly[4,8-bis-(2-ethylhexyloxy)-benzo[1,2-b:4,5-b']dithiophene-2,6-diyl-alt-(4-(2-ethylhexanoyl)-thieno[3,4-b]thiophene))-2,6-diyl] (PBDTTT-C) and Phenyl-C70-butyric acid methyl ester (PC70BM) with a weight ratio of 1:1.5. The additive diiodooctane (DIO) is used with ratios between 0% and 10% to increase the compatibility of the two components. We investigate the surface structure of the devices with amplitude modulation atomic force microscopy (AFM). Conventional AFM height and phase images are complemented with data obtained from maps of amplitude-phase-distance (APD) curves. This allows us to determine the unperturbed (true) surface and the mechanical properties of the soft surface layer of the specimen. The AFM height and phase images of PBDTTT-C:PC70BM blends produced with different ratio of DIO indicate, that the additive plays a fundamental role in the structure formation process. Blends with DIO ratios between 1.8% and 5% show the best power conversion efficiency (PCE) up to 6.9%. We discuss the structure and the structure of the interface between donor and acceptor components in view of their impact on charge carrier dynamics and solar cell performance.

CPP 31.13 Wed 16:30 Poster C

Triplet Excitons and Cations in DCV4T-Me:C₆₀ blends with different mixing ratio — ●DANIEL SCHÜTZE¹, CHRISTIAN KOERNER¹, ROLAND FITZNER², EGON REINOLD², PETER BÄUERLE²,

KARL LEO¹, and MORITZ RIEDE¹ — ¹Institut für Angewandte Photophysik, Technische Universität Dresden, Germany — ²Institut für Organische Chemie II und Neue Materialien, Universität Ulm, Germany

Dicyanovinyl end-capped oligothiophenes (DCVnT) have demonstrated their ability of achieving high power conversion efficiencies of up to 6.9% in a bulk heterojunction solar cell¹. Besides that, they act as a model system because of the possibility of changing properties by varying the length of backbone or side chains.

In this work, we use DCV4T with two methyl side chains at the first and the last thiophene ring. By photoinduced absorption spectroscopy (PIA) measurements we probe the long-living (μ s-ms) excited states (triplet excitons, cations) after photoexcitation of our samples. With PIA, their generation and recombination behavior can be investigated. Here, we report our results obtained on a series of DCV4T-Me:C₆₀ blends with varying mixing ratio from 3:1 to 1:2. We found strong influence of the mixing ratio on the generation rate of triplet excitons and also an influence in the generation rate and the activation energy of free charge carriers with increasing temperature. The results are compared to solar cells containing identical blend layers as active layer to investigate the dependence of the photo current on the mixing ratio.

¹ Fitzner et al., J. Am. Chem. Soc. 2012, 134, 11064 (2012)

CPP 31.14 Wed 16:30 Poster C

Nucleation and Growth of Copper Phthalocyanine from Solution — ●FATEMEH GHANI and HANS RIEGLER — Max Planck Institute f. Colloid & Interfaces, Potsdam-Golm, Germany

Silver nanoparticles are usually synthesized by physical vapor deposition or through complicated methods like ion implantation or wet chemistry. A self-assembly method is of interest due to its simplicity and cost-efficiency [202]. By combining physical vapor deposition and solvent treatment (spin casting), We applied a simple hybrid method to produce ap-proprate silver nanoclusters for organic solar cells. Through evaporation of the silver film (\sim 5 nm), nanoclusters (of \sim 4 nm height and \sim 25 nm widths) cover the surface. By spin casting the solvent, a thin liquid film covers the evaporated film. The silver clusters redistribute in the solution film and by evaporation of the solvent, they aggregate in larger clusters (\sim 20 nm height and \sim 45 nm width). The process is influenced via physical parameters of growth from solution like evaporation rate and liquid film concentration. We show that the size of the clusters can be controlled by the thickness of the deposited film, type of solvent, and spin casting speed. We applied this method to increase the efficiency of a hybrid solution processed and vacuum deposited unsubstituted copper phthalocyanine/fullerene organic solar cells.

CPP 31.15 Wed 16:30 Poster C

Charge generation in solid-state dye-sensitized solar cells using peryleneimide sensitizers — ●YOOJIN KIM, MICHAEL MEISTER, IAN HOWARD, FELIX HINKEL, GLAUCO BATTAGLIARIN, CHEN LI, KLAUS MÜLLEN, and FRÉDÉRIC LAQUAI — Max Planck Institute for Polymer, Mainz, Germany

Solid-state dye-sensitized solar cells (DSCs) have attracted a lot of attention owing to their advantages compared to liquid-electrolyte DSCs such as ease of fabrication and the absence of corrosive electrolytes that are typically used in liquid-electrolyte cells. However, fast charge recombination between electrons in the titania nanoparticle films and dye/hole conductor cations, incomplete pore-filling, and the decreased thickness of titania films necessary for efficient charge extraction currently limit the power conversion efficiency. In this contribution we compare the charge generation and recombination processes in a series of peryleneimide-sensitized DSCs studied by steady-state photoinduced absorption (PIA) and ultrafast broadband transient absorption spectroscopy (TAS) covering the sub-picosecond to millisecond timerange. By fitting the dynamics to a photophysical model we extract the parameters relevant for the photovoltaic efficiency such as the yield of electron injection and the recombination rate constants which allows us to derive meaningful structure-property relations.

CPP 31.16 Wed 16:30 Poster C

Sequentially solution-processed bulk-heterojunction CuPc/PCBM - bilayer for organic solar cells — ●MARKUS REGNAT, FATEMEH GHANI, and HANS RIEGLER — Max Planck Institut of Colloids and Interfaces, Potsdam-Golm, Germany

Copper Phthalocyanine (CuPc) is a commonly used electron donor material in vacuum-processed organic solar cells (OSC) due to its suitable

electronic properties, chemical stability and low material cost. Recent studies have revealed appropriate solvents for CuPc [1] and thus also opened a way for cost-efficient wet-deposition techniques, like spin casting or dip coating. Based on this, a working hybrid solution/vacuum processed OSC with a CuPc film prepared by wet-processing (spin cast) could be obtained [2]. The nanostructures of the CuPc film have an important influence on the efficiency of the OSC. A systematic study reveals the impact of various process parameters on nucleation and growth of wet-processed CuPc films and allows the optimization of the nanostructures. By using appropriate orthogonal solvents, even both essential optoelectronic layers (CuPc, PCBM) can now be sequentially wet-deposited for a bulk-heterojunction CuPc/PCBM - bilayer OSC.

[1] Ghani, F.; Kristen, J.; Riegler, H., Solubility properties of unsubstituted metal phthalocyanines in different types of solvents, *J. Chem.* (2012)

[2] Fatemeh Ghani; Ivelin Bochukov; Konstantinos Fostropoulos; Hans Riegler, Hybrid solution/vacuum-processed bilayer heterojunction organic solar cells: Structural characterization and performance, *Thin Solid Films* (2012)

CPP 31.17 Wed 16:30 Poster C

Preferential orientation of molecular dipoles in amorphous vacuum deposited films studied by surface potential measurements — ●CHRISTIAN WEIGEL, SAMI HAMWI, and WOLFGANG KOWALSKY — Institut fuer Hochfrequenztechnik, TU Braunschweig

Amorphous thin films of semiconducting small molecules are commonly used in organic optoelectronic devices to avoid detrimental effects of grain boundaries in polycrystalline thin films. Studies of surface potential development with film thickness have shown that sublimation of common OLED molecules such as Tris(8-hydroxyquinolino) aluminum (Alq3) or 1,3,5-tris(2-N-phenylbenzimidazolyl)benzene (TPBi) results in amorphous films with a preferential orientation of the molecular dipoles. Kelvin probe measurements provide a sensitive tool to detect a shift in the average molecular dipole orientation by as little as 5 degrees from the isotropic case. The detected shift in surface potential is characteristic for each molecule and is found in the order of several volts per 100 nm, comparable to operating voltages of organic electronic devices. The recorded increase in surface potential is largely independent of material or preparation of the substrate upon which the amorphous film is grown (barring the different interface dipoles between substrate and film), so that anisotropy at the organic film to vacuum interface drives the preferential orientation. Upon optical excitation, the measured potential vanishes, presumably due to mobile charges screening the dipole field.

CPP 31.18 Wed 16:30 Poster C

Encapsulation of small molecule organic devices by a functional thin top layer of tetratetracontane — ●FLORIAN STAUB¹, ANDREAS STEINDAMM^{1,2}, MICHAEL BRENDEL^{1,2}, and JENS PFLAUM^{1,2} — ¹Experimental Physics VI, Julius-Maximilians-University, 97074 Würzburg — ²ZAE Bayern, 97074 Würzburg

Providing long-term stability for organic devices is still a challenging task due to the sensitivity of molecular materials as well as organic/metal interfaces on water incorporation and oxidation processes. The straight-chain alkane tetratetracontane (TTC) is capable to protect organic devices from those degradation mechanisms by forming closely packed and highly crystalline films [1]. TTC is transparent in the visible range, highly hydrophobic and chemically inert and therefore suited to conserve the opto-electronic properties of the underlying films. In this contribution we apply nanometer thick top layers of TTC by thermal vacuum deposition onto planar heterojunction organic photovoltaic cells (OPVCs) based on zinc phthalocyanine (ZnPc) and diindenoperylene (DIP) in combination with the acceptor C₆₀, respectively. For ensuring best comparability, encapsulated and bare cells are prepared under identical conditions on the same substrate. We investigate the degradation mechanisms by measuring the external quantum efficiency and the IV-characteristics over time under exposure to various environmental conditions (vacuum, nitrogen, air). The occurring changes in the opto-electronic device performance will be discussed in relation with structural data obtained by AFM and X-ray diffraction. [1] M. Göllner et al., *Adv. Mater.* 2010, 22, 4350-4354

CPP 31.19 Wed 16:30 Poster C

Brightly Blue and Green Emitting Copper Compounds for Singlet Harvesting in OLEDs — ●MARKUS LEITL¹, FRITZ-ROBERT KÜCHLE², LARS WESEMANN², and HARTMUT YERSIN¹ — ¹Institut für Physikalische und Theoretische Chemie, Universität Re-

gensburg, D-93040, Germany — ²Institut für Anorganische Chemie, Universität Tübingen, D-72076, Germany

In this contribution, a series of four Cu(I) complexes is presented. All substances exhibit high emission quantum yields of up to 65 % at relatively short emission decay times of several μ s. The emission wavelength varies from the blue (460 nm) to the green (505 nm). This is induced by defined modifications of the chemical structure. Detailed photophysical investigations reveal that the energy separation $\Delta E(S_1 - T_1)$ between the triplet state T_1 and the singlet state S_1 is small and lies in the range of 500 cm^{-1} . As a consequence, emission at ambient temperature originates dominantly (> 99 %) from the S_1 state which is thermally populated from the energetically lower lying T_1 state. For this reason, the emission at ambient temperature represents a thermally activated delayed fluorescence (TADF). It is proposed to utilize this property for collecting both singlet and triplet excitons in the lowest excited singlet state for light generation in OLEDs. This effect represents the singlet harvesting mechanism.

CPP 31.20 Wed 16:30 Poster C

Interface trap density investigation by impedance spectroscopy of MIS structures for different surface treatments — ●HIPPOLYTE HIRWA, STEVE PITTNER, and VEIT WAGNER — Jacobs University bremen, Campusring 1, D-28759 Bremen, Germany

For high performance electronic devices, reliability and stability are crucial parameters. Since reliabilities and stabilities issues in field effect transistors are mainly related to the semiconductor-gate insulator interface properties, a MIS (Metal-insulator-semiconductor) capacitor structure can be equally used for investigation of interface traps. We report on impedance measurements carried out on MIS capacitors fabricated using silicon oxide as insulator prepared under 3 different surface treatments and poly(3-hexylthiophene) as semiconductor. The conductance technique was used to extract the interface trap density. For this a proper equivalent circuit for our MIS structures had to be chosen. The results reveal first the formation of a double layer with 2 different conductivities in the semiconductor layer, secondly the presence of interface trap states and finally they show that the interface states density and energy distribution is related to the sample surface treatment.

CPP 31.21 Wed 16:30 Poster C

Combined photoemission and X-ray absorption study of the 'rods-in-belt' supramolecular complexes containing gold-copper and gold-silver clusters — ●ANNA MAKAROVA^{1,2}, ELENA GRACHOVA², DMITRY KRUPENYA², JULIA SHAKIROVA², IGOR KOSHEVOY³, ECKART RÜHL⁴, CLEMENS LAUBSCHAT¹, SERGEY TUNIK², and DENIS VYALIKH¹ — ¹Technische Universität Dresden, Dresden, Germany — ²St.-Petersburg State University, St.-Petersburg, Russia — ³University of Joensuu, Joensuu, Finland — ⁴Freie Universität Berlin, Berlin, Germany

Recently created self-assembled Au(I)-Cu(I) and Au(I)-Ag(I) 'rods-in-belt' supramolecular complexes display intriguing phosphorescence properties. Another important issue is the tunability of their electronic structure, and consequently their photophysical properties through modification of the ligand environment that opens great perspectives for their implementation in light-emitting devices and in bio-imaging. It is believed that high structural ordering and self-assembling properties of such objects can open a new avenue for the design of artificial nanostructures that may potentially be ideal building blocks for next generation electronics. Nonetheless, the electronic structure of these materials has not been investigated experimentally by now. We have demonstrated that photoemission and X-ray absorption techniques can be successfully applied for systematic investigation of the series of these unique complexes. It has been shown that the all complexes inside the series exhibit similar electronic structures, however, the electronic states near the HOMO reveal notable differences.

CPP 31.22 Wed 16:30 Poster C

A multiscale modeling study of loss processes in block-copolymer-based solar cell nanodevices — ●SERGIJ DONETS, ANTON PERSHIN, and STEPHAN BAEURLE — University of Regensburg, Institut of Physical and Theoretical Chemistry, D-93053

Flexible photovoltaic devices possess promising perspectives in optoelectronic technologies, where high mobility and/or large-scale applicability are important. However, their usefulness in such applications is currently still limited due to the low level of optimization of their performance and durability. For the improvement of these properties a

better understanding and control of small-scale annihilation phenomena of the elementary particles involved in the photovoltaic process, such as exciton loss and charge carrier loss, are necessary. Here, we explore the causes for their occurrence with a novel field-based solar-cell algorithm on the example of self-organizing nanostructured block-copolymer systems, which possess a broad variability in their chemical and physical characteristics, and explore new routes to optimize their performance. From our calculations, we deduce that in the regime from

low up to intermediate χ -parameters the charge transport efficiency (CTE) and internal quantum efficiency (IQE) of both block-copolymer systems increase up to a maximum, characterized by a minimum in the number of charge losses due to charge recombinations. In the regime of high χ -parameters they form nanostructures with a large number of bottlenecks and dead ends, leading to a large number of charge losses due to charge recombination, charge trapping and an impaired exciton dissociation.

CPP 32: Poster: Organic Semiconductors

Time: Wednesday 16:30–18:30

Location: Poster C

CPP 32.1 Wed 16:30 Poster C

Organic Magneto-optoelectronics: Magnetoresistive Organic Field-Effect Transistors — •THOMAS REICHERT, CAROLIN ISENBERG, TOBAT SARAGI, and JOSEF SALBECK — Macromolecular Chemistry and Molecular Materials (mmCmm), Department of Mathematics and Science and Center for Interdisciplinary Nanostructure Science and Technology (CINSA-T), University of Kassel, Heinrich-Plett-Strasse 40, 34132, Kassel, Germany.

In organic semiconductors the spin-correlation between quasiparticles can be influenced by low magnetic fields, which leads to large (up to 20% at 10mT) magnetoresistance at room temperature. This organic magnetoresistance (OMAR) is not only highly interesting for addressing fundamental questions about spin-transport and spin-manipulation in organic materials, but also for the realization of lightweight, flexible, multifunctional magneto-optoelectronic applications. We were able to develop different types of magnetoresistive organic field-effect transistors (OFETs) and present an overview about the corresponding magnetic-field dependent effects (Photoinduced magnetoresistance; Magnetoresistance based on donor/acceptor blends; Photoinduced sign change of magnetoresistance) as well as the underlying fundamental physical processes. These results do not only pave the way for the application of organic semiconductors in future multifunctional magneto-optoelectronic devices but also help to identify the details of spin-dependent processes in organic semiconductors.

CPP 32.2 Wed 16:30 Poster C

Self-aggregation of fullerene derivatives in water: a molecular dynamics simulation study — •SRINIVASA RAO VARANASI¹, OLGA GUSKOVA¹, ANDREAS JONN¹, PETER FRIEDEL¹, and JENS-UWE SOMMER^{1,2} — ¹Leibniz Institute of Polymer Research, Dresden, Germany — ²TU Dresden, Dresden, Germany

Some of the amphiphilic derivatives of fullerene are known to self-assemble in solution at the nanoscale into various shapes (spherical, rod-like and vesicle depending on the length of the side chain, functionality of the substituent, concentration and temperature). This self-aggregation behaviour seems to determine their photophysical as well as photochemical activities. The understanding of self-aggregation behaviour in water is not only useful in photovoltaic applications but also in biomedical applications (for example, effects on lipid membranes). We present here a molecular dynamics simulation study on amphiphilic fullerene derivatives in water. We used PCFF force field along with Girifalco's parameters for modeling fullerene derivatives and TIP3P model for water. In this study, we analyze various structural and dynamic properties related to fullerene derivatives as well as water.

CPP 32.3 Wed 16:30 Poster C

Charge generation and loss processes in polymer-polymer solar cells — •HANNAH MANGOLD¹, IAN A. HOWARD¹, MARCEL SCHUBERT², DIETER NEHER², and FRÉDÉRIC LAQUAI¹ — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²Institute of Physics, University of Potsdam, Germany

All-polymer solar cells, where both donor and acceptor component are π -conjugated polymers, have the advantage of a broad absorption over the entire visible wavelength range. In this contribution we use broadband visible and near-infrared transient absorption spectroscopy covering the picosecond to microsecond timescale to investigate the charge generation and loss processes in various blends of the well-known donor polymer P3HT with a naphthalenediimide (NDI)-based copolymer exhibiting maximum power conversion efficiencies up to 1.4%. We demonstrate that the anticorrelation between the NDI-aggregation and solar cell performance recently reported by us [1] is

caused by a variation of the fraction of contact sites between the donor and acceptor polymer that can facilitate free charge generation and that this fraction is strongly influenced by the choice of solvents used for film preparation. [1] Schubert et al, *Adv. Energy Mat.* 2012, 2, 369.

CPP 32.4 Wed 16:30 Poster C

Linear X-ray dichroism of perylene diimide derivatives and its correlation with their transport properties — •NINA ZEILMANN¹, SUSANNE BACKES², BENEDIKT RÖSNER¹, ANDREAS SPÄTH¹, KATRIN LUDWIG¹, ANDREAS HIRSCH², and RAINER H. FINK¹ — ¹FAU Erlangen-Nürnberg, Physical Chemistry II and ICMM, Erlangen, Germany — ²FAU Erlangen-Nürnberg, Organic Chemistry II and ZMP, Erlangen, Germany

The development of organic semiconductors for organic electronic applications has undergone notable progress during the last years. While hole transporting p-type semiconductors have already shown performances comparable to their inorganic analogues, competitive electron transporting n-type materials still pose a challenge. Among these materials, perylene diimide derivatives are very promising and interesting candidates. Since the transport properties are often strongly correlated with the microstructure of the organic films, microscopic probes that provide high chemical specificity and sensitivity to molecular orientation at high spatial resolution are required. Scanning transmission X-ray microspectroscopy (STXM) ideally combines these requirements. Within this contribution we present a microspectroscopic analysis of thin films of various perylene diimide derivatives prepared on Si₃N₄ membranes. Polarization dependent light microscopy gives clear evidence on the growth of large domains with preferential molecular orientations. Using STXM, film and orientational homogeneities can directly be correlated with the electronic transport properties. The project is funded by the BMBF, contract 05K10WEA.

CPP 32.5 Wed 16:30 Poster C

Structural Aging and Degradation of Polymer Solar Cells — •CHRISTOPH SCHAFER¹, JAN PERLICH², STEPHAN V. ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹Technische Universität München, Physik-Department - Lehrstuhl Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching — ²HASYLAB at DESY, Notkestr. 85, 22607 Hamburg

One of the major challenges in OPV is to elongate their lifetimes. Several mechanisms of organic solar cell degradation have been proposed in literature within the last years. Most of the mechanisms are related to chemical alteration of the applied materials, such as photo-bleaching and oxidation of the active organic layer and the metal contacts or the diffusion of oxygen or water into the organic layer. However, insufficient research has been done on determining transitions of the nanomorphology of the active layer of bulk heterojunction (BHJ) polymer solar cells as an effect of aging. These transitions are expected to strongly affect the properties of solar cells since the active layer morphology plays a crucial role in the energy conversion process. In our investigations, we study the influence of illumination on the morphology of the active layers of PCPDTBT:PC71BM solar cells. Therefore, advanced scattering techniques such as grazing incidence small angle x-ray Scattering (GISAXS) are performed both in-situ on operating PCPDTBT:PC71BM solar cells and ex-situ on pre-aged polymer-blend films. The findings are supplemented with UV/Vis and characteristic IV curve measurements.

CPP 32.6 Wed 16:30 Poster C

The influence of processing additives on the morphology of bulk heterojunction films — •WEIJIA WANG¹, MARTINE

PHILIPP¹, DAVID MAGERL¹, JEAN-FRANCOIS MOULIN², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany — ²HZ Geesthacht at FRM II, Lichtenbergstr.1, 85748 Garching, Germany

In the last decades, photoactive polymers and its applications in organic photovoltaic have attracted tremendous attention. Compared with standard inorganic solar cells, there are plenty of advantages for these materials, such as light weight, easy processibility and low cost. Currently the main drawback is still the low efficiency. It is already observed that the morphology of the heterojunction film plays an important role in organic solar cells. In this work, in order to modify the morphology, different amount of additives are applied in blend system rrP3HT:C61-PCBM. The internal structure is investigated with grazing incidence small angle neutron scattering (GISANS) in time-of-flight (TOF) mode. Additionally, the surface morphology is probed with optical microscopy and atomic force microscopy. The effect on molecular level is investigated by absorption.

CPP 32.7 Wed 16:30 Poster C

Systematic investigation on ternary bulk heterojunction solar cells based on PTB7:PC70BM — ●CHRISTIAN JENDRZEJSKI, SHUAI GUO, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany

Organic solar cells hold great promise for future applications in photovoltaics as they have several advantages, like the potentially lower production costs, much lower weight and flexibility in comparison to inorganic solar cells. In the present investigation the new, high efficient chlorobenzene based PTB7:PC71BM bulk heterojunction system are prepared and investigated with the addition of different third components. These kind of ternary systems have shown a promising result, which combines the advantages of the host material as well as the third component, and therefore improves the final power conversion efficiency. The inner structure of the ternary blend films is probed via X-ray reflectivity (XRR) and grazing incidence small angle X-ray scattering (GISAXS). The surface morphology is investigated with atomic force microscopy (AFM) and scanning electron microscopy (SEM). Via integrating XRR, GISAXS, AFM and SEM data, the inner 3D structure of the ternary films is obtained. As a consequence, the correlation between the nano-morphology of the films and the efficiency of the polymer-based solar cells is addressable.

CPP 32.8 Wed 16:30 Poster C

Molecular orientation and growth mode of organic molecular beam deposited ultrathin HBC films on SiO₂ — ●PAUL BEYER^{1,2}, TOBIAS BREUER³, SALIOU NDIAYE³, GREGOR WITTE³, and STEFAN KOWARIK² — ¹Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — ²Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — ³Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg, Germany

Hexa-peri-hexabenzocoronene (HBC) is a polycyclic aromatic hydrocarbon that is investigated in supramolecular electronics due to its high electron mobility of up to $1\text{cm}^2/\text{Vs}$. We examine the real-time growth kinetics of organic molecular beam deposited ultrathin HBC films on silicon dioxide using x-ray diffraction and x-ray spectroscopy.

With grazing incidence x-ray diffraction (GIXD) we observe a larger crystallinity at higher substrate temperatures of 150°C but rough films. We observe smooth films as indicated by growth oscillations of specular x-ray reflectivity (XRR) during growth of HBC at lower temperatures of 25°C . The growth oscillations show changes in the molecular arrangement during the first monolayers. To test whether the molecular orientation changes we use near edge x-ray absorption fine structure (NEXAFS) spectroscopy at the BESSY II synchrotron. NEXAFS is used to determine the orientation of the π^* orbitals and therefore the orientation of the HBC molecules in (sub)mono- and multilayer films. We find that the molecules on average are tilted by an angle of 74° relative to the surface plane.

CPP 32.9 Wed 16:30 Poster C

Vibronic spectra of excitons in 2-D polyacene lattices — ●CHRISTOPH WARNS¹, THOMAS HARTMANN¹, IVAN LALOV^{2,1}, and PETER REINEKER¹ — ¹Institute for Theoretical Physics, Ulm University, 89069 Ulm, Germany — ²Faculty of Physics, Sofia University, Sofia 1164, Bulgaria

Vibronic spectra of excitons in various 2-dimensional lattices, which

model the (ab)-plane of polyacene crystals, have been investigated. We have considered interacting FEs and molecular vibrations, taking into account linear and quadratic coupling. The linear optical susceptibility of the 2-D crystal was calculated using the Green's function method and the vibronic approach. Various 2-D crystal lattices were assumed: actual anthracene, tetracene and pentacene crystal lattices, a hypothetical graphene-like lattice, all with two molecules per unit cell, and a simple hexagonal lattice with only one molecule per unit cell. In the computation of the vibronic spectra we used the measured excitonic and vibrational parameters of polyacene crystals (based on data by Petelenz et al.).

CPP 32.10 Wed 16:30 Poster C

Aggregate Structures and Electron Transport Anisotropy in High Mobility n-type Low Bandgap Copolymer — ●ROBERT STEYRLEUTHNER¹, RICCARDO DI PIETRO¹, SCOTT HIMMELBERGER², BRIAN COLLINS³, FRANK PALZER⁴, HOLM KIRMSE⁴, MARCEL SCHUBERT¹, ZHIHUA CHEN⁵, HARALD ADE³, ALBERTO SALLES², ANTONIO FACCHETTI⁵, and DIETER NEHER¹ — ¹University of Potsdam, Institute of Physics — ²Stanford University, Materials Science and Engineering — ³North Carolina State University, Department of Physics, — ⁴Humboldt University Berlin, Institute of Physics — ⁵Polyera Corporation, Illinois

We have recently explored the photophysics of the high electron mobility ($0.85\text{cm}^2/\text{Vs}$) conjugated copolymer P(NDI2OD-T2), also known as Polyera ActivInk N2200. From these studies we could estimate, that approx 45% of the polymer chains in thin films exist in an aggregated (π -stacked) conformation mainly independent of the preparation routine [1]. However, special solvents mixtures can induce changes of the orientation and the molecular structure of the chain aggregates which we prove by GIXD and TEM measurements. We further investigate the structure property relation by correlating the morphology with the electron transport anisotropy in P(NDI2OD-T2). [1] R. Steyrleuthner et al., J. Am. Chem. Soc., 2012, 134 (44)

CPP 32.11 Wed 16:30 Poster C

Understanding changes in optical absorption of thin organic films during growth — INES TRENKMANN¹, CHRISTOPHER KEIL², DERCK SCHLETTWEIN², and ●HARALD GRAAF¹ — ¹nanoMA (Center for nanostructured Materials and Analytics), Chemnitz University of Technology, D-09107 Chemnitz, Germany — ²Institute of Applied Physics, Justus-Liebig-University Giessen, D-35392 Giessen, Germany

The optical absorption of organic thin films changes during growth. Here mainly the lowest energy transition shows a red shift with increasing film thickness. Different explanations are given in the literature: e.g. increasing island sizes leading to larger coupled systems [1] or a change in the ratio between the numbers of molecules in the bulk compared to surface molecules [2]. We investigated three perylene derivatives showing all the expected red shift of the lowest energy transition. They are characterized by different morphologies and growth modes: One shows a layer-by-layer growth and two (an amorphous and a crystalline) show island growth. The shift for the layer-by-layer perylene can be explained by a combination of the two above mentioned explanation. The shift for the first approximately 1.5 monolayers can be understood by a two-dimensional island growth with increase of coupled chromophoric systems. Further film growth lead to an increase of the ratio between the number of molecules in the bulk with respect to the surface molecules. For the other two molecules the experimental results on the red-shift can be explained by a new theoretical model.

[1] Chau et al. J.Phys.Chem 97 (1993) 2699, [2] e.g. Heinemeyer et al. Phys.Rev.Lett. 104 (2010) 257401

CPP 32.12 Wed 16:30 Poster C

Optoelectronic Processes in Squaraine Dye-Doped OLEDs for Emission in the Near-Infrared — ●B. STENDER¹, S. F. VÖLKER², C. LAMBERT², and J. PFLAUM^{1,3} — ¹Experimental Physics VI, University of Würzburg, D-97074 Würzburg — ²Institute of Organic Chemistry and Center for Nanosystems Chemistry, University of Würzburg, D-97074 Würzburg — ³ZAE Bayern, D-97074 Würzburg

Organic light-emitting diodes (OLEDs) for emission in the near-infrared (NIR) offer the great advantage of room temperature operation due to inherently high exciton binding energies (several 100 meV) in contrast to their inorganic counterparts. Despite several approaches have been presented with reasonable efficiency, purely organic NIR-emitters are barely investigated due to degradation of the organic compound. To cope with this challenge a novel organic host-guest system consisting of the polymer SY-PPV and the squaraine

dye monomer M has been investigated. Optical excitation reveals a highly efficient energy transfer from the visible range to the NIR (750 nm) with a doping concentration of less than 2.0 wt.% and an associated Förster radius of 3.8 nm. As will be demonstrated, electrically driven NIR-emission yields an efficiency of 0.65% at a current density of 2.26 mA/cm² with a turn-on voltage of 2.0 V at a doping concentration of only 0.05 wt.%. Comparison between steady-state photo- and electroluminescence provides access to the opto-electronic processes on molecular length scales, thereby indicating that NIR-OLED emission in this system is controlled by charge carrier dynamics rather than by exciton transfer.

CPP 32.13 Wed 16:30 Poster C

Modeling Mesoscale Morphology of Polymeric Semiconductors using Soft Models — ●PATRICK GEMÜNDEN^{1,2}, CARL PÖLCKING¹, KURT KREMER¹, DENIS ANDRIENKO¹, and KOSTAS DAOULAS^{1,2} — ¹Max-Planck-Institut für Polymerforschung, Mainz, Germany — ²InnovationLab GmbH, Heidelberg, Germany

Polymeric semiconductors are characterized by hierarchical structuring where the mesoscopic morphology is affected by details of molecular architecture and interactions. Here we will discuss a strategy for developing models for the description of these materials by combining systematic coarse-graining with phenomenological descriptions. As a case study we will consider a model for P3HT systems where each bead corresponds to a single hexylthiophene unit. The bonded interactions are obtained from underlying atomistic configurations using the VOTCA package. The non-bonded interactions are captured by combining soft isotropic and orientation-dependent potentials. The former controls the equation of state of the material in the amorphous state while the latter leads to liquid-crystalline mesophases with a stack-like structuring.

Using the above model, Monte Carlo simulations of systems with device-relevant dimensions (\sim 50 nm) were performed. We will discuss the effect of the molecular weight on the morphology. The conformations of the polymer chains for stack-like structuring will be analyzed and related to charge transport properties.

CPP 32.14 Wed 16:30 Poster C

Morphological aspects of the exciton transport in thin films of Diindenoperylene — ●ALEXANDER STEEGER¹, ANNA KATHARINA TOPCZAK¹, and JENS PFLAUM^{1,2} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²ZAE Bayern, 97074 Würzburg

The exciton diffusion length (EDL) is a key criterion for an optimized design of organic thin film devices. As a tight correlation between

morphology and charge carrier as well as exciton transport properties has been evidenced in previous studies, the extension of crystalline domains has been proposed beneficial for long range exciton transport [1]. To address this point we have varied the morphology of Diindenoperylene (DIP) thin films by means of the substrate temperature (T_S). X-ray diffraction analysis revealed an almost amorphous phase of DIP grown at $T_S = 100$ K, whereas $T_S = 300$ K and 400 K yield to long range ordered polycrystalline films of higher crystallinity with increasing T_S . Photoluminescence-quenching measurements together with an advanced modeling were performed to correlate the EDL to the DIP morphology. Long range ordered DIP layers grown at $T_S = 300$ K and 400 K show a high EDL (59 nm and 115 nm, respectively), whereas the EDL of DIP deposited at $T_S = 100$ K is significantly smaller. This result emphasizes the importance of long range structural order to achieve superior transport properties of photo-generated electron-hole pairs. Financial support by the DFG focus program SPP 1355 is gratefully acknowledged. [1] R. R. Lunt et al., Adv. Mater 22 (2010) 1233-1236

CPP 32.15 Wed 16:30 Poster C

Determination of molecular transition dipole orientation of organic emitters by angular-dependent photoluminescence measurements — ●CHRISTIAN MAYR, TOBIAS SCHMIDT, BERT SCHOLZ, LARS JÄGER, and WOLFGANG BRÜTTING — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Organic light-emitting diodes (OLEDs) have been investigated for more than 20 years and are standing now at the frontier to mass production. Current research focuses on the enhancement of light outcoupling efficiency which is reduced especially due to the energy dissipation to surface plasmons (SPs). Numerical simulations show that a horizontal emitter orientation with respect to the substrate can enhance the efficiency by up to 50% due to reduced coupling to SPs. 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 not only makes it possible to study molecular orientation in neat thin films but also of small amounts of emitters doped into a matrix material without knowing any detailed information of the optical properties of the dopant. Hence, this method is particularly useful for the investigation of newly developed materials. The method is applied to Iridium-based phosphorescent emitters in order to gain a consistent efficiency analysis of OLEDs and possibilities to enhance light outcoupling.

CPP 33: Poster: Charged Soft Matter

Time: Wednesday 16:30–18:30

Location: Poster C

CPP 33.1 Wed 16:30 Poster C

Why is the partition coefficient of some ionic liquids concentration-dependent? — ●AXEL ARNOLD^{1,3}, DIRK REITH^{2,3}, and THORSTEN KÖDDERMANN³ — ¹Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany — ²Bonn-Rhein-Sieg University of Applied Studies, Sankt Augustin, Germany — ³Fraunhofer-Institute for Algorithms and Scientific Computing (SCAI), Sankt Augustin, Germany

The partition coefficient of a substance measures its solubility in octanol compared to water, and is frequently used as a rough estimate of toxicity. If a substance is hardly soluble in octanol, it is practically impossible for it to enter (human) cells, and therefore is less likely to be toxic. While for simple substances, the partition coefficient is concentration-independent, this is not true for a few important classes of complex molecules, such as ionic liquids or tensides.

We present a simple model for the partition coefficient of ionic liquids based on the association and dissociation of ion pairs. Using solvation free energies in water and octanol from computer simulations, this model can reproduce the partition coefficient of the commonly used ionic liquid 1-Butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide [C₄MIM][NTf₂] for a wide range of concentrations. Our findings show that the concentration dependence of the partition coefficient is mostly an entropic effect due to the strong tendency of the ionic liquid to associate in water, but dissociate in oc-

tanol.

CPP 33.2 Wed 16:30 Poster C

Coupling of surface charge and pH effects: charge inversion and reentrant condensation in protein solutions with multivalent cations — ●FELIX ROOSEN-RUNGE¹, BENJAMIN HECK¹, FAJUN ZHANG¹, OLIVER KOHLBACHER², and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik, Universität Tübingen — ²Zentrum für Bioinformatik, Universität Tübingen

Charge regulation of proteins is a fundamental mechanism in biological systems, depending on the pH of the solution and condensation of counterions. We report on charge inversion and the related reentrant phase behavior in solutions of globular proteins with different multivalent metal cations [1,2], addressing the coupling of pH effects and charge regulation. For several proteins and both acidic and neutral metal salts, charge inversion as measured by electrophoretic light scattering is found to be a universal phenomenon, whose extent depends on the specific protein-salt combination. Reentrant phase diagrams show a much narrower phase-separated regime for acidic salts. The experimental findings are reproduced with good agreement by an analytical model accounting for ion condensation, pH effects due to metal hydrolysis and charge regulation of side chains. Using a DLVO picture, reentrant phase behavior can be explained. Finally, the relation of charge inversion and reentrant condensation is discussed, suggesting that pH variation in combination with multivalent cations provides

control of both attractive and repulsive interactions between proteins.

- [1] F. Zhang, et al., *Soft Matter* 8 (2012) 1313
 [2] F. Zhang, et al., *PRL* 101 (2008) 148101

CPP 33.3 Wed 16:30 Poster C

Using Super-Heterodyne Laser Doppler Velocimetry for measurements in low concentration suspensions of charged colloids — ●BASTIAN SIEBER and THOMAS PALBERG — Institut für Physik, Johannes Gutenberg Universität Mainz, Staudingerweg 7, D 55122 Mainz

Soft condensed matter is characterized both by its softness and an internal structure on a mesoscopic scale. This allows convenient optical access to system structure and dynamics in equilibrium. Among the various soft matter systems, charge stabilized colloidal dispersions have gained recognition as tremendously useful model condensed matter systems because of their structural ordering and rich phase behaviour. Experimentally, we studied electrokinetic flow in closed cells with electroosmotic solvent flow. Super heterodyning renders the data of interest free of homodyne contributions and low frequency noise. We used this method to study an aqueous charged sphere suspension driven under the influence of an external electric field. Measurements have been performed on suspensions of various concentrations by diluting the suspension further between measurements to reach very low concentrations in the process. Preliminary results show an increase in the electro-osmotic velocity with lower concentration while the electrophoretic velocity is decreasing. Further data on this topic will be provided and discussed.

CPP 33.4 Wed 16:30 Poster C

Small differences with big impact: Reentrant phase behavior induced by multivalent cations in protein solutions — ●MARCELL WOLF, FAJUN ZHANG, FELIX ROOSEN-RUNGE, and FRANK SCHREIBER — Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

Subtle difference between proteins can lead to remarkably big differences in their resulting behavior. Using a multivalent cation, yttrium chloride (YCl_3), a reentrant condensation (RC) with a liquid-liquid phase separation (LLPS) within the condensed regime has been established in a negatively charged protein system [1,2]. Here we compare the phase behavior of two serum albumins, BSA and HSA. They are highly similar in the primary structure but the comparison between the RC behavior of these two albumins shows that minor differences in the primary protein structure have a strong influence on such a system. The range of the condensed regime is much broader for HSA. Optical microscopy also shows a shift of the LLPS region to lower salt and protein concentrations in the case of HSA, where the LLPS region is much broader. The formation of clusters in the condensed regime and outside the LLPS region is systematically studied by SAXS, SLS/DLS and we observe that the cluster size is much smaller by using HSA. Differences of the primary structure between the two proteins leads to changes in the hydrophobicity and charge distribution of the proteins. These changes in BSA and HSA phase diagrams can be related to differences in protein structure. [1] F. Zhang et al., *PRL* 101, 2008, 148101; [2] F. Zhang et al., *Soft Matter* 8, 2012, 1313.

CPP 33.5 Wed 16:30 Poster C

Thin films of lithium containing block copolymer electrolyte — ●SIMON BRUNNER¹, EZZELDIN METWALLI¹, MARTIN BAUMANN¹, WILLIAM HEFTER¹, MAN NIE¹, VOLKER KÖRSTGENS¹, JAN PERLICH², STEPHAN V. ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany — ²HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany

In the light of an increasing demand on power sources for portable electronic devices, nano-scaled lithium based membranes pave the way for new opportunities regarding design, application and integration of rechargeable batteries. In this work, thin hybrid films [1] based on block copolymer electrolytes and lithium salt are investigated using grazing-incidence small angle x-ray scattering (GISAXS) and real space techniques such as SEM, AFM and optical microscopy. In both bulk and thin film format of the lithium-polymer nanocomposite, lithium ions were found to prevent the crystallization of PEO and an enhanced micro-phase separation is observed as evident by both SAXS and GISAXS investigations. Probes of lithium containing thin films sandwiched between two metal electrodes were prepared and the film conductivity is measured using impedance spectroscopy. The effects of salt concentration and membrane morphology on the ionic conductiv-

ity are demonstrated.

- [1] E. Metwalli, M. Nie, V. Körstgens, J. Perlich, S.V. Roth, P. Müller-Buschbaum, *Macromol. Chem. Phys.* 212, 1742-1750 (2011).

CPP 33.6 Wed 16:30 Poster C

Adsorption Behavior of Oppositely Charged Polyelectrolyte/Surfactant Mixtures: Neutron Reflectivity from Alkyltrimethylammonium Bromides (CTABs) and poly[tris(hydroxymethyl)methylacrylamide (PAMPS) mixtures at the Air/Water Interface — ●HEIKO FAUSER, NORA KRISTENHOCHREIN, MARIN UHLIG, and REGINE VON KLITZING — Technische Universität Berlin, 10623 Berlin, Deutschland

If a polyelectrolyte and a surfactant of opposite charge are mixed, the two ions associate forming a large variety of complexes. Different interfacial adsorption behavior leads to different foaming properties.

Former studies done in our group on mixtures of the negatively charged polyelectrolyte PAMPS with the positively charged CTAB revealed a different adsorption behavior in foam film lamellas and at the air-water interface.

To gain a detailed insight into the structure and composition of the film interfaces, we performed neutron reflectometry measurements at the air/water interface.

Our approach focusses on a fixed surfactant concentration while varying the amount of polyelectrolyte. In order to get information about the composition and layer structure we investigated mixtures of different isotopic contrast. Also the influence of different surfactant chain lengths (C12,C14) and variation in electric charge of the polyelectrolytes are investigated.

CPP 33.7 Wed 16:30 Poster C

Charge transport and electrode polarization at the interface between glass forming ionic liquids (ILs) and metal electrodes — ●LUDWIG POPP, CIPRIAN GHIORGHITA IACOB, WYCLIFFE KIPROP KIPNUSU, MARTIN TRESS, JOSHUA RUME SANGORO, and FRIEDRICH KREMER — Institute of Experimental Physics I, Leipzig, Germany

Charge transport and electrode polarization phenomena are investigated in a homologous series of imidazolium-based ionic liquids by broadband dielectric spectroscopy (BDS) in a large temperature (190 - 300 K) and frequency range ($10^{-3} - 10^5$ Hz). The dielectric spectra are dominated – on the low frequency side – by electrode polarization, while, for higher frequencies, charge transport (in a disordered matrix) is the underlying physical mechanism. The absolute values of dc conductivity vary over 5 decades upon systematic variation of ILs structure and electrode material. A microscopic model is applied to quantitatively describe the electrode polarization. The applicability of the model to the experimental data in a broad frequency range is discussed in more details [1-4].

References: [1]. Serghei, A. et al. (2009), *Phys. Rev. B*, 80(18), 184301-5, [2]. Dyre, J. C. (1988), *Phys. Rev. B*, 37(17), 10143-10149, [3]. Sangoro, J. R., Ph.D. Thesis, (2010), University of Leipzig, [4]. Kremer, F., Schönhals, A. (2003), *Broadband Dielectric Spectroscopy*, Springer, Berlin.

CPP 33.8 Wed 16:30 Poster C

Manning condensation on DNA fragments with monovalent and divalent counterions — ●DAMIR VURNEK^{1,2}, MARIJA SORIĆ², and TOMISLAV VULETIĆ² — ¹Institut für Theoretische Physik and Cluster of Excellence: EAM, Universität Erlangen-Nürnberg, Erlangen, Germany — ²Institut za fiziku, Zagreb, Croatia

We obtained the Manning free (uncondensed) counterions fraction θ for dilute aqueous solutions of rodlike polyions: 150 bp DNA fragments, across a range of concentrations, $c(\text{monomer}) = 0.03 - 8$ mM. Conductometric measurements were done on Na^+ DNA and Mg^{++} DNA, in 1mM added salt (NaCl and $MgCl_2$, respectively) as well as in pure water conditions.

We remind that the high linear charge of polyions Manning condenses a fraction of counterions close to the polyion. This partly neutralizes polyion charge, and reduces the effective solution conductivity. Our conductivity study of DNA in added salt confirms theoretical values $\theta = 0.24$ and 0.12 for Na^+ DNA and Mg^{++} DNA, respectively. However, in pure water conditions, towards lower DNA concentrations the effective θ increases well above the Manning values. UV-absorbance measurements showed that this is not due to DNA denaturation. Denaturation may occur in pure water conditions due to a reduction in the electrostatic screening; as single stranded DNA has a lower linear charge it also has a correspondingly higher θ fraction. We concluded that in dilute solutions more counterions must become

decondensed as the entropy gain overcomes the electrostatic cost, as Deshkovski et al. (Phys.Rev.Lett. 2001) indeed have discussed.

CPP 33.9 Wed 16:30 Poster C

The effects of reactive oxygen species on single polycation layers — ●FLORIAN BERG¹, STEPHAN BLOCK², STEFFEN DRACHE¹, RAINER HIPPLER¹, and CHRISTIANE A. HELM¹ — ¹Inst. für Physik, Uni Greifswald, D-17487 Greifswald — ²ZIK HIKE, D-17487 Greifswald

Positively charged, branched polyethylenimine (PEI) adsorbed onto silicon wafers are attacked by free hydroxyl radicals. With AFM Colloid Probe technique, the surface forces between the PEI layers are measured. The force profiles show that freshly deposited PEI layers are flat, i.e., electrostatic repulsion dominates the interaction. After radical attack both, surface potential and surface charge density, are reduced by a factor of about two, while the Debye length remains unchanged. Force volume measurements show a homogeneous distribution of the surface charge on the μm scale. To probe the nm-scale, negatively charged gold nanoparticles (NP) are adsorbed. After radical attack we find a 10 % decrease of saturation coverage consistent with the decreased surface charge density if the electrostatic three-body interaction is considered. Nevertheless, the NP adsorption kinetics is slowed down suggesting that the PEI-layer is inhomogeneous on the nm-scale after radical attack.

CPP 33.10 Wed 16:30 Poster C

Polyelectrolytes Adsorbed onto Oppositely Charged Lipid Monolayers - Reduced Charge Densities — THOMAS ORTMANN¹, ●HEIKO AHRENS¹, ANDREAS GRÖNING¹, FRANK LAWRENZ¹, ANDRE LASCHEWSKY², and CHRISTIANE A. HELM¹ — ¹Inst. für Physik, Uni Greifswald, D-17487 Greifswald — ²Fraunhofer Institute for Applied Polymer Research, Potsdam-Golm, Germany

Polyelectrolytes in dilute solutions (10^{-5} monoMol/L) adsorb in a two-dimensional lamellar phase to oppositely charged lipid monolayers at the air/water interface. To investigate the influence the electrostatic interaction, a statistic copolymer with 90% and 50% charged monomers and mixtures between charged and uncharged lipids are used. With grazing incidence diffraction the separation between stretched polyelectrolyte chains is determined. The monomer/lipid ratio is calculated. When the fraction of charged monomers is reduced to 50%, the chain distance decreases from 4.5nm to 3nm (at an area per lipid of 80\AA^2) i.e. less than proportional and the ratio of lipids to charged monomers decreases from 0.7 to 0.5. Similarly, when the fraction of charged lipids is decreased the distance of the polyelectrolyte chains is increased sub-proportionally.

CPP 33.11 Wed 16:30 Poster C

Quaternized Brushes of Weak Polyelectrolytes (PE): Brush Structure Studied with Neutron Reflectometry — ●ZULEYHA YENICE¹, JAN GENZER², REGINE V.KLITZING¹, and RALF KÖHLER^{1,3} — ¹Stranski Lab, Inst. of Chemistry, TU Berlin, Germany — ²Dept. of Chemical & Biomolecular Engineering, NCSU, Raleigh, USA — ³Inst. of Soft Matter and Functional Materials, HZB Berlin, Germany

PE-brushes are used for surface modifications because of properties as specific adsorption, permeability and stimuli responsive behavior. PDMAEMA* is a weak PE with pH-dependent properties, giving room for further modifications like protonizing by varying the pH, or turning them into strong PE by quaternization. The PDMAEMA-brush was gradually quaternized with deuterated iodomethane. Deuterium simultaneously labels the brush for neutron reflectometry (NR) without altering its chemistry. NR was applied to detect the inner structure, density, and thickness after partially quaternizing the brush, to see the iodide distribution in the brush, lateral and vertical to the substrate. First results indicate an increase of the iodide content at the surface in lateral direction what is paralleled by an increase of brush thickness. Up to now, the vertical distribution of iodide is still unclear but is probed by incorporation of charged gold nanoparticles (Au-NP) along the charge gradient. Penetration depth and distribution of deposited Au-NP was investigated with ellipsometry. Specular and off-specular NR will be used to determine possible internal structures to clarify the potential of PE-brushes as functionalized substrate and as tool for nano-templating. *poly[2-(dimethylamino) ethyl methacrylate]

CPP 33.12 Wed 16:30 Poster C

Polyelectrolyte Multilayers (PEM) of different charge densities in humid atmospheres: Structural changes and swelling mechanics — INGO DÖNCH¹, PATRICK OTT², ANDRÉ LASCHEWSKY²,

ANDREAS FERY³, RUMEN KRASTEV⁴, and ●RALF KÖHLER^{1,5} — ¹Interfaces, MPI-KGF Potsdam/Golm — ²Applied Polymer Chemistry, University of Potsdam — ³Physical Chemistry II, University of Bayreuth — ⁴Biomaterials, NMI at University of Tübingen — ⁵Soft Matter and Functional Materials, HZB Berlin: Germany

PEM consist of complexed layers of two organic polyions of opposite charge build-up by layer-by-layer deposition. They are known for a high tunability of their structural properties, e.g. thickness and roughness on nanoscale. The interplay of internal interactions and structure of PEM is investigated by means of swelling experiments, i.e. an internal mechanical stress in the films is induced by incorporation of solvent molecules from adjacent solvent vapour (H₂O). Neutron reflectometry is used to test for structure parameters of the sample and its specific material content of polymer and solvent. Three different PEM systems made from PSS/PDADMAC* by spraying technique are investigated; each containing a derivative of the polycation PDADMAC of 75, 89, or 100% charge density (ChD) along the molecular chain, also the number of adsorbed layers of polyions, i.e. the film thickness, is varied. The swelling characteristics changes continuously and systematically with the number of adsorbed bilayers indicating internal transitions of structure and swelling. Lower ChD results in thicker films. * poly-(styrene sulphonate)/ poly-(diallyldimethyl ammonium)

CPP 33.13 Wed 16:30 Poster C

The structure of fluids with impurities — ●MARKUS BIER and LUDGER HARNAU — Max Planck Institute IS, Stuttgart, Germany, and University of Stuttgart, Germany

The influence of dilute impurities on the structure of a fluid solvent is investigated theoretically. General arguments, which do not rely on particular models, are used to derive an extension of the Ornstein-Zernike form for the solvent structure factor at small scattering vectors. It is shown that dilute impurities can influence the solvent structure only if they are composed of ions with significantly different sizes. Non-ionic impurities or ions of similar size are shown to not alter the solvent structure qualitatively. This picture is compatible with available experimental data. The derived form of the solvent structure factor is expected to be useful to infer information on the impurity-solvent interactions from measured scattering intensities.

Reference:

[1] M. Bier and L. Harnau, Z. Phys. Chem. **226**, 807 (2012).

CPP 33.14 Wed 16:30 Poster C

molecular dynamics simulations of polyelectrolyte brushes under poor solvent conditions — ●GUILI HE¹, HOLGER MERLITZ², and JENS-UWE SOMMER¹ — ¹Leibniz-Institut fuer Polymerforschung Dresden, 01069 Dresden, Germany — ²Department of Physics and ITPA, Xiamen University, Xiamen 361005, P.R. China

Molecular dynamics simulations have been applied to investigate salt-free planar polyelectrolyte brushes under poor solvent conditions with respect to the molecular backbone under the variation of the chain degree of polymerization, the brush grafting density and the charge fraction (strength of the electrostatic interaction). We found that, with decreasing the system temperature (changing solvent quality) far below the theta point, the brush first displays lateral phase separation with respect to the solvent and eventually collapses vertically [see also J.-M. Y. Carrillo and A. V. Dobrynin, Langmuir 2009, 25(22)]. The lateral phase separation leads to cylindrical morphologies (bundles of chains) which has been observed for different charge fraction, degree of polymerization and grafting density. Even changing the size and solvent selectivity of the counterions cannot prevent lateral structure formation in the poor solvent state. This phenomenon can be explained by an entropy gain of counterions in the cylindrical state as compared to the homogeneously collapsed state at the same temperature.

CPP 33.15 Wed 16:30 Poster C

Charge and Mobility of Polyelectrolyte Complex Nanoparticles — KARSTEN GELFERT, UWE LAPPAN, SIMONA SCHWARZ, and ●ULRICH SCHELER — Leibniz-Institut für Polymerforschung Dresden e.V.

Polyelectrolyte Complex nanoparticles formed from poly(maleicanhydride-coethylene) and poly(diallyldimethylammonium chloride) have been studied by a combination of NMR, EPR and light scattering under variation of the overall composition of the complexes. Dynamic light scattering and PFG NMR yield complementary information on the hydrodynamic size, where PFG NMR is more sensitive to primary complexes and DLS to the nanoparticles. The importance of primary

particles for the total stability of the system has been shown. Electrophoresis NMR permits the measurement of the effective charge of both the primary complexes and nanoparticles. In conjunction with the NMR spectroscopic on the chemical species involved, free polyelectrolytes are excluded all excess material is contained in pri-

mary complexes. Selective placements of spin labels on the polyanion permits the investigation of molecular dynamics by EPR lineshape analysis showing strong hinderance of teh local mobility in the minority component.

CPP 34: Poster: Wetting, Micro and Nano Fluidics

Time: Wednesday 16:30–18:30

Location: Poster C

CPP 34.1 Wed 16:30 Poster C

3D-Velocimetry by Photonic Rutherford Scattering — ●MARKUS SELMKE and FRANK CICHOS — Universität Leipzig, molecular nanophotonics

We propose of a new kind of 3D-velocimetry using absorbing nanoparticles and a variant of photothermal single particle microscopy. Using a Quadrant photodiode detector we reveal that photons are deflected by a photonic potential which is created by a local refractive index change around a laser-heated absorbing nanoparticle. The deflection experienced is shown to be the analog to the deflection of a massive particle wave-packet in unscreened (spin-less) Coulomb scattering, i.e. the quantum mechanical analog to Rutherford Scattering. The experimentally found focal detection geometry reveals an adjustable lateral split sub-volume feature which allows new (cross-) correlation-based 3D-velocimetry experiments of absorbing particles with ultra-high sensitivity.

CPP 34.2 Wed 16:30 Poster C

Genie in a Channel — ●STEFAN REUTTER — TU Darmstadt

When high-energy heavy ions are shot at a thin sample ($< 100 \mu\text{m}$), they leave a large number of parallel ion tracks. These can be etched to obtain mesoscopic cylinders with a narrow diameter distribution whose mean can be varied between 30 nm and 1 μm .

These channels can then be filled with a liquid to investigate properties such as diffusion and phase behaviour when trapped in a volume small enough that confinement effects become significant, but at the same time large enough that surface effects do not have a dominating influence on liquid dynamics.

I will present the results of diffusometry measurements on simple liquids and binary liquid systems in ion track channels obtained by Static Field Gradient Echo NMR experiments.

CPP 34.3 Wed 16:30 Poster C

Faster than spinodal dewetting: Ultra-thin liquid polystyrene films on silanized Si wafers — ●MATTHIAS LESSEL¹, OLIVER BÄUMCHEN², MARKUS RAUSCHER³, and KARIN JACOBS¹ — ¹Department of Experimental Physics, Saarland University, D-66041 Saarbrücken, Germany — ²Department of Physics and Astronomy, McMaster University, Hamilton, ON, Canada L8S 4M1 — ³Max Planck Institute for Intelligent Systems, Heisenbergstr. 3, D-70569 Stuttgart, Germany

In recent years, many studies showed that a thin liquid film on a solid surface in air bears more complexity than expected from a simple three-layer-system: e.g. a highly mobile surface layer in case the liquid is an unentangled polystyrene (PS) melt (Yang et al., Science 2010; Seemann et al., J. of Polym. Sci. 2006) or a nearly full slip boundary condition for the PS melt on a solid substrate (Bäumchen et al., PRL 2009). Our study focuses on such phenomena and explores their influence on dewetting. We use hydrophilic and -phobic Si wafers, either covered by a highly ordered silane self-assembled monolayer or by a thin layer of an amorphous fluoropolymer. On each of the substrates, one expects for a certain set of parameters spinodal dewetting for the PS melt (Seemann et al., PRL 2001). However, contrary to expectations, we observed a thermally activated nucleation process of hole formation instead of spinodal dewetting. The observed behavior is similar to results on free standing polymer films (Croll et al., Macromolecules 2012). A theory based on the capillary model of Croll et al. taking the effective interface potential into account will be presented to describe the results.

CPP 34.4 Wed 16:30 Poster C

Advanced in situ GISAXS investigations of drying and adsorption kinetics — ●BERIT HEIDMANN^{1,2}, MATTHIAS SCHWARTZKOPF¹, GONZALO SANTORO¹, SHUN YU¹, GERD

HERZOG^{1,2}, ROMAN MANNWEILER¹, JOHANNES F.H. RISCH¹, WILFRIED WURTH², and STEPHAN V. ROTH¹ — ¹Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, D-22607 Hamburg, Germany — ²Universität Hamburg, Institut für Experimentalphysik, Luruper Chaussee 149, 22761 Hamburg, Germany

Tailored gold nanoparticle assemblies play an important role for technological applications like solar cells, nanocatalysts and bioelectronics [1]. Solution casting is a promising process that enables low-cost fabrication of such devices. Grazing incidence small-angle X-ray scattering (GISAXS) is a powerful tool for in situ investigations of fast surface processes on nanoscale [2]. We have combined GISAXS and a contact angle apparatus to perform drop drying kinetic measurements with improved accuracy and flexibility. Using advanced drop casting deposition technique, we investigated in situ the drying kinetics during self-assembly of gold nanoparticles and the influence of different functionalized silicon surfaces on the process. In order to investigate the effect of the X-ray beam on sample surfaces, we compared in situ and ex situ drop drying experiments. Furthermore, the setup allows for investigation of different wetting behaviors as a function of X-ray radiation dose. [1] Bauer et al., Nanotechnology, 14, 1289-1311 (2003) [2] Roth et al., J. Phys.: Condens. Matter, 23, 254208 (2011)

CPP 34.5 Wed 16:30 Poster C

Forced Displacement Experiments in quasi 2D Porous Media. — ●MICHAEL JUNG^{1,2}, MARTA SANCHEZ DE LA LAMA², DANIEL HERDE², STEPHAN HERMINGHAUS², MARTIN BRINKMANN^{1,2}, and RALF SEEMANN^{1,2} — ¹Universität des Saarlandes, Saarbrücken, Germany — ²Max Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany

As a model for a forced liquid displacement process into porous media, we study two-dimensional flow experiments in microfluidic devices. The devices and the porous structures are fabricated from oil-resistant UV-curable glue using soft-lithography. The devices were first saturated with oil (silicon oils, fluorinated oils or alkanes) and subsequently the oil was displaced by either a volume or pressure controlled water flush. We observe the global and local dynamic behavior of the advancing liquid fronts and the residual oil distribution using high speed microscopy as function of wettability, viscosity, flow velocity, and geometry of the pore space. On the length scale of individual pores we also investigate the influence of pressure fluctuations, which occur when a liquid front invades a throat. These experimental results are compared to numerical simulations based on multiple particle collisions for analogous pore geometry and wetting conditions.

CPP 34.6 Wed 16:30 Poster C

A new approach to measure the Depth of Correlation in micro-PIV — ●MICHAEL HEIN¹, BERNHARD WIENEKE², and RALF SEEMANN^{1,3} — ¹Department of Experimental Physics, Saarland University, Saarbrücken, Germany — ²LaVision GmbH Göttingen, Germany — ³MPI for Dynamics and Self-Organization, 37073 Göttingen, Germany

In recent years micro-particle image velocimetry (micro-PIV) has become the most frequently used tool to measure flow profiles in microfluidics. Micro-PIV uses volume-illumination and imaging of fluorescent tracer particles through a microscope objective. The velocity-vectors are obtained by correlating two images captured shortly after each other. Thus the obtained velocity field depends on all imaged particles within an interrogation window, even on the defocused particles. Accordingly, the system dependent knowledge of the height extension of the measured plane (Depth of Correlation, DOC) is crucial when considering three dimensional flow profiles. We present a novel approach to determine the DOC based on artificial volume data derived with the same optical setup as used for the experiments. Using this method we examine the DOC in dependence of out-of-plane velocity

gradients for commonly used microscope objectives.

CPP 34.7 Wed 16:30 Poster C

X-ray photon correlation spectroscopy (XPCS) study of nanospheres in parabolic microflow — ●RAPHAEL URBANI¹, FABIAN WESTERMEIER², BERND STRUTH², and THOMAS PFOHL¹ — ¹Chemistry Department, University of Basel, 4056 Basel, Switzerland — ²HASYLAB, Deutsches Elektronen-Synchrotron, 22607 Hamburg, Germany

The combination of state-of-the-art microfluidics with small angle X-ray scattering (SAXS) and X-ray photon correlation spectroscopy (XPCS) has been successfully used for dynamic investigations of colloidal particles in microflow with different geometric constraints.

Using a coherent X-ray beam of small size (about $10\ \mu\text{m} \times 10\ \mu\text{m}$) allows us to measure static and dynamic properties at different spatial positions within in the microfluidic channel system. We are able to measure autocorrelation functions at fixed q -positions in the range of 10^{-6} - 10^{-1} s with an APD-detector and simultaneously at a wide q -range in a temporal range of 4×10^{-3} - 10^2 s using a 2D fast readout detector. Analyzing the autocorrelation functions, we obtain detailed information about advective and diffusive transport within the microfluidic flow of different velocities and in different channel geometries such as curvatures and constrictions.

By means of the combination of XPCS with microfluidics we probe spatially dependent the influence of microfluidic velocity fields, shear stress, hydrodynamic (wall) interactions and inertia effects on the transport behavior of the nanoparticles.

CPP 34.8 Wed 16:30 Poster C

Microfluidic Platform for Membrane Fusion Studies — ●NABOR VARGAS¹, JEAN-BAPTISTE FLEURY¹, and RALF SEEMANN^{1,2} — ¹Experimental Physics, Saarland University, D-66041 Saarbrücken — ²MPI for Dynamics and Self-Organization, D-37073 Göttingen

Membrane fusion is essential for the life of eukaryotic cells, it is known as the process whereby two separate lipid bilayers merge to become one by means of a family of fusogenic proteins. Research on membrane fusion has been intense along past decades, but we are still far from unveiling the whole phenomena. We are exploring a new microfluidic approach to study single membrane fusion events in a controllable geometry. This experimental setup shall allow for the production of stable lipid bilayers, easy variation of the lipid membrane composition like the insertion of proteins, and superior control of the fusion process by e.g. by optical and electrical access. Lipid bilayers created inside the microfluidic chip can be moved and manipulated making them interact with each other resembling cell membrane fusion.

CPP 34.9 Wed 16:30 Poster C

Gold nanostructure assisted thermophoretic trapping of single nano-objects — ●MARCO BRAUN and FRANK CICHOS — Institute for Experimental Physics I, University of Leipzig, Linnéstraße 5, D - 04103 Leipzig

The manipulation and trapping of nano-objects that undergo Brownian motion are of great interest in soft-matter sciences. Optical tweezing is the most common technique for the trapping of individual particles in solution and is based on the optical gradient force. Hence, a sufficiently high polarizability of the particle in the solution is required. While it is thus easy to trap single dielectric particles larger than 100 nm, a trapping of smaller objects such as single molecules by means of optical tweezers can hardly be realized. Molecular trapping can be achieved by a technique called Anti-Brownian Electrokinetic trap (ABEL trap), which exploits the feedback controlled electric field of four electrodes. Hence, the latter technique requires electrical contacts, which introduce difficulties when fabricating multiple traps. Here, we present an all-optical technique which replaces the electric fields by highly localized thermal fields. The so-called thermophoretic trap exploits thermophoretic forces that act on a particle placed in a temperature gradient, which e.g. locally distorts the screening of the surface charges and by that induce a particle drift. In our approach the temperature field is generated by an optically heated Au nanostructures. Due to the small dimensions of the heat sources, even a small temperature increase introduces large temperature gradients causing a strong thermophoretic drift by which the motion of a diffusing particle can be manipulated.

CPP 34.10 Wed 16:30 Poster C

Imaging of drops on superhydrophobic surfaces in the Cassie and Wenzel states — ●PERIKLIS PAPAIOPOULOS, LENA MAMMEN,

XU DENG, DORIS VOLLMER, and HANS-JÜRGEN BUTT — Max Planck Institute for Polymer Research, Mainz, Germany

A droplet deposited or impacting on a superhydrophobic surface rolls off easily, leaving the surface dry and clean. This remarkable property is due to a surface structure which favors the entrainment of air cushions beneath the drop, leading to the so called Cassie state. The Cassie state competes with the Wenzel (impaled) state, where the liquid fully wets the substrate. To utilize superhydrophobicity, impalement of the drop into the surface structure needs to be prevented. Recently, we demonstrated the capability of laser scanning confocal microscopy (LSCM) to image water drops on an array of micropillars [1]. While the drop evaporates from a pillar array, its rim recedes via step-wise depinning from the edge of the pillars. Once the pressure becomes too high, or the drop too small, the drop slowly impales the texture. The thickness of the air cushion decreases gradually. As soon as the water-air interface touches the substrate, complete wetting proceeds within milliseconds. LSCM opens a novel approach to study wetting dynamics, which is of high scientific and technological interest.

[1] P. Papadopoulos *et al.*, *Langmuir* **2012**, *28*, 8392-8398

CPP 34.11 Wed 16:30 Poster C

Effect of Wettability on Water-Oil Front Progression in Porous Media — ●ALEN KABDENOV^{1,2}, HAGEN SCHOLL¹, KAMALJIT SINGH^{2,3}, MARCO DI MICHEL³, MARIO SCHEEL³, STEPHAN HERMINGHAUS², and RALF SEEMANN^{1,2} — ¹Saarland University, Experimental Physics, D-66041 Saarbrücken, Germany — ²Max Planck Institute for Dynamics and Self-Organization, D-37073 Göttingen, Germany — ³European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble, France

The effect of wettability on the three dimensional water-oil front progression in an initially oil filled porous medium during a water flood is observed in situ using ultrafast synchrotron X-ray tomography. The wettability of the porous media was controlled by using different cleaning and coating procedures, using different bead material or by using a variety of combinations of experimental fluids. It is shown that for smaller contact angles, the front progresses in a compact shape without any oil trapping and a single pore-volume of water flood is sufficient to reach the final state. By contrast, the front roughens in the case of larger contact angles, and forms several enlarged fingers due to front stopping at smaller throats. These fingers bypass several oil filled pore-pockets leading towards significant oil trapping and water flooding of more than three pore-volumes is required to achieve the final oil distribution. The trapped oil ganglia remain in place due to strong interfacial forces which is difficult to overcome in the tested regime of small capillary numbers.

CPP 34.12 Wed 16:30 Poster C

Laser interferometric observations of capillary rise in arrays of silicon nanochannels — ●MARK BUSCH, FELIX KOCH, and PATRICK HUBER — Hamburg University of Technology, Hamburg, Germany

We present measurements on the capillary filling of nanochannels in mesoporous silicon films with organic solvents, polymers and epoxy resins. The time-dependent rise level of the liquids within the channels has been determined with laser interferometry [1]. This allows us to analyze the filling process with a high temporal (milliseconds) and spatial (micrometer) resolution. We found distinct changes in the imbibition dynamics as a function of the filling direction, from the top to the bottom or from the bottom to the top of the film. These peculiarities will be discussed with respect to a gradient in the porosity and/or a monotonic variation in the mean channel diameter as a function of channel length.

[1] L. Acquaroli *et al.*: Capillary Filling in Nanostructured Porous Silicon, *Langmuir* **27** (2011), No. 5, p. 2069-2072

CPP 34.13 Wed 16:30 Poster C

Structure and Dynamics in Hydrophilic Confinement from First Principles — ●CHRISTOPH ALLOLIO, TOBIAS WATERMANN, and DANIEL SEBASTIANI — Institute of Chemistry, Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 4, 06120 Halle (Saale)

Geometric confinement has a strong effect on water, making it quite different from the bulk.[1] To understand e.g. protein agglomeration, and folding, it is necessary to develop a better understanding of water under confinement.

We investigate the anomalous behavior and hydrogen bond network

of water molecules confined at various interfaces using ab-initio molecular dynamics and spectroscopy. In addition to structural data, we use proton NMR chemical shifts as a measure for the strength of the hydrogen-bonding network. Our calculations illustrate the modifications of the ^1H NMR chemical shifts of confined water with respect to bulk water.[2] In the vicinity of silanols, weakly hydrogen bonded liquid water is observed, while at greater distances the hydrogen bonding network is enhanced with respect to bulk water. In addition we analyze the dynamics, finding e.g. a considerable slowing down of water diffusion at a water silica interface.

[1] N. Giovambattista, P. J. Rossky, P. G. Debenedetti, *Annu. Rev. Phys. Chem.* **63** (2012), 179.

[2] X. Y. Guo, T. Watermann, S. Keane, C. Allolio, D. Sebastiani, *Z. Phys. Chem.* **226** (2012), 1415.

CPP 34.14 Wed 16:30 Poster C

Fouling layer removal investigations under cross-flow conditions — ●GERD HERZOG^{1,2}, ADELIN BUFFET¹, MATTHIAS SCHWARTZKOPF¹, GUNTARD BENECKE^{1,3}, FRANS J. DE JONG⁴, VOLKER KÖRSTGENS⁵, KUH SARKAR⁵, PETER MÜLLER-BUSCHBAUM⁵, WILFRIED WURTH², and STEPHAN V. ROTH¹ — ¹HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg — ²Universität Hamburg, Institut für Experimentalphysik, Luruper Chaussee 149, D-22761 Hamburg — ³MPI of Colloids and Interfaces, Department of Biomaterials, Am Mühlenberg 1, D-14476 Potsdam-Golm — ⁴TU Hamburg-Harburg, Institut für Mehrphasenströmungen (V-5), Eißendorfer Straße 38, 21073 Hamburg — ⁵TU München, Physik-Department E13, James-Frank-Str. 1, 85748 Garching

The process of scaling and fouling under cross-flow conditions as well as the removal of deposit layers is important for many technical applications like membranes, heat exchangers and ship hull coatings.

We used grazing incidence small-angle X-ray scattering (GISAXS) and a microfluidic cell for an in-situ investigation of the removal of an annealed polystyrene colloid layer on a glass substrate under a flow of deionized water. The sample was scanned several times in horizontal direction and the obtained data show the continuous transition from a polymer-covered to a pure glass substrate.

CPP 34.15 Wed 16:30 Poster C

Study of the interface of droplets using pH change — ●BIRTE RIECHERS, QUENTIN BROUSSEAU, FLORINE MAES, and JEAN-CHRISTOPHE BARET — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Interfaces are prevalent in many systems such as emulsions and foams. They can be stabilized using surfactant molecules. Amphiphilic molecules influence the properties of the interface (e.g. surface tension, interfacial rheology) as well as the bulk properties of the two phases (e.g. pH). The understanding of these properties is fundamental for the control of emulsion encapsulation for biological compartmentalization [Baret, *Lab Chip* 12 (2012), 422; Baret et al., *Langmuir* 25 (2009), 6088].

In our study, the effect of surfactants on the pH inside the droplets of emulsions is investigated. We combined a microfluidic fluorescence setup with a pH sensitive dye to monitor pH changes with time. Ionic surfactant molecules are dissolved in the continuous phase and upon adsorption to the interface release protons into the dispersed phase. Our results regarding the change of pH inside the droplets will bring quantitative information on interfacial surfactant coverage and thus allowing to conclude the stability of the interface for microencapsulation.

CPP 34.16 Wed 16:30 Poster C

Acoustic Sorting of Drops and Cells — ●LOTHAR SCHMID¹ and THOMAS FRANKE^{1,2} — ¹Universität Augsburg, Experimentalphysik I, Soft Matter Group, Augsburg, Germany — ²Department of Physics and School of Engineering and Applied Science, Harvard University, Cambridge, USA

We use a surface acoustic wave (SAW) device for manipulating fluids, droplets and cells in microfluidic channels.

The acoustic wave is coupled into the channel at specific regions, generating pressure gradients or microvortices. Electric control of the wave generator allows for precise regulation and fast switching times.

We show an application of the technique by demonstrating a microfluidic fluorescence-activated sorter for cells and droplets at high rates. Our acoustic sorter combines the advantages of traditional fluorescence-activated cell sorting (FACS) and droplet sorting (FADS)

and is applicable to a multitude of objects. We can sort aqueous droplets at rates as high as several kHz into two or more outlet channels. We demonstrate cell sorting in one-phase flow using fibroblasts cells without prior encapsulation into drops directly from the bulk phosphate buffered saline media. Our acoustic micro-FACS meets conventional laboratory practice but at the same time allows for modular integration into more complex microfluidic setups.

CPP 34.17 Wed 16:30 Poster C

Nonlinear chemical reactions in a droplet — ●MARIA SCHWARZL, ROBERT NIEDL, IGAL BERENSTEIN, and CARSTEN BETA — Institute of Physics and Astronomy, University of Potsdam, Germany

Over the last decade, microfluidic systems with water in oil droplets have developed into a widely used design principle for chemical and biological applications. In particular, the use of droplets as small micro-reactors has stimulated enormous research activities. Among other aspects, the mixing behavior inside such droplets has been a topic of wide interest. It was observed that inside a droplet, aqueous solutions with different viscosities may exhibit faster mixing as compared to components with equal viscosity. Related to this observation, we have found that a nonlinear clock reaction, when operated in a linear microfluidic channel, can be accelerated by using fluids of different viscosities. To further characterize the effects that are responsible for these observations, we compare measurements of enzymatic and inorganic autocatalytic reactions in linear microchannels with those measured in a droplet system.

CPP 34.18 Wed 16:30 Poster C

Hydrogel driven microfluidics in structured paper substrates — ●ROBERT NIEDL and CARSTEN BETA — Institute of Physics and Astronomy, University of Potsdam, Germany

Many clinical tests require a purified analyte in combination with freshly prepared biological solutions. Under working conditions far away from standard clinical laboratories, e.g. in developing countries, such prerequisites are often difficult to establish. Here, we present a system that offers a solution to such problems. We extend the recently developed concept of paper-based microfluidics by incorporating a hydrogel into the paper device. The swollen hydrogel stores a defined volume of fluid on the sensor substrate. Through a thermally driven collapse of the hydrogel, the liquid is released to drive the fluidic system without any pumps or other sophisticated equipment. Sensitive chemicals deposited in initially dry sections of the paper substrate can be dissolved and transported across fluidic channels imprinted in the paper substrate. In this way, different chemicals can be supplied in a well-controlled and timely fashion to a reaction area, in which a specific assay may be performed. We demonstrate this concept by implementing a standard glucose test in this type of hydrogel-driven paper-fluidic device.

CPP 34.19 Wed 16:30 Poster C

The interplay of capillary rise and vapour phase adsorption in nanoporous Vycor glass — ●SEBASTIAN KIEPSCH, NICO BOHR, and ROLF PELSTER — FR 7.2, Experimentalphysik, Universität des Saarlandes, Campus E2.6, D-66123 Saarbrücken, Germany

The spontaneous imbibition of polar organic liquids, primarily n-decanol ($\text{C}_{10}\text{H}_{21}\text{OH}$), has been studied for nanoporous Vycor glass by means of dielectric spectroscopy. Vycor glass is an interconnected pore network with pore diameters $d_p \approx 7.5$ nm and volume porosity $\Phi \approx 35\%$. For large times t , the imbibition dynamics can be described by the Lucas-Washburn law, $h(t) = c_h \sqrt{t}$. Here, h denotes the capillary height and the prefactor c_h depends on fluid parameters (viscosity, surface tension) and matrix parameters (porosity, radius ...). However, during the initial phase of the process, a systematic deviation from the square root behaviour occurs. We address the question whether the imbibition dynamics are a simple superposition of capillary rise and concurrent vapour phase adsorption. The time dependence of the latter process is measured in a controlled environment using the same technique.

CPP 34.20 Wed 16:30 Poster C

Capillary Levelling of Stepped Polymer Films - A Nanofluidic Probe of the Slip Boundary Condition — ●OLIVER BÄUMCHEN¹, THOMAS SALEZ², JOSHUA D. MCGRAW¹, MICHAEL BENZAQUEN², PAUL FOWLER¹, ELIE RAPHAËL², and KARI DALNOKI-VERESS¹ — ¹Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, L8S 4M1 — ²Laboratoire de Physico-Chimie Théorique, UMR CNRS

Gulliver 7083, ESPCI, Paris, France

For flows on small length scales, the hydrodynamic boundary condition of a liquid at a solid surface plays an enormous role. In recent years much has been learned about this slip boundary condition from flows that are driven by internal, capillary, forces such as dewetting of thin liquid films. For the case of dewetting, holes in the film grow, driven by exposing the underlying substrate. Here, we present the opposite approach: We show that the capillary levelling of initially curved surfaces, in our case stepped polymer films, is sensitive to the nano-rheological properties of the liquid [1] and the slip boundary condition at the buried liquid/substrate interface. A thin film model which includes the hydrodynamic boundary condition enables us to quantify slip at the buried interface and to extract its dependence on the molecular weight of the polymer.

[1] J.D. McGraw, T. Salez, O. Bäümchen, E. Raphaël, and K. Dalnoki-Veress, *Physical Review Letters* 109, 128303 (2012).

CPP 34.21 Wed 16:30 Poster C

Theory of water and charged liquid bridges — ●KLAUS MORAWETZ — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP) Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

The phenomena of liquid bridge formation due to an applied electric field is investigated. The effect of electromagnetic fields on a charged catenary is described by a new solution which allows to determine the static and dynamical stability conditions where charged liquid bridges are possible. The creeping height, the bridge radius and length as well as the shape of the bridge is calculated showing an asymmetric profile in agreement with observations. The flow profile is calculated from the Navier Stokes equation leading to a mean velocity which combines charge transport with neutral mass flow and which describes recent experiments on water bridges.

AIP Advances 2 (2012) 022146, *Phys. Rev. E* 86 (2012) 026302

CPP 34.22 Wed 16:30 Poster C

Early stages of nanoparticle attachment to polyelectrolyte layers - in-situ GISAXS investigations with microfluidics and dipcoating — ●VOLKER KÖRSTGENS¹, DAVID MAGERL¹, NEELIMA

PAUL¹, MARTINE PHILIPP¹, JAN PERLICH², STEPHAN V. ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany — ²HASYLAB at DESY, 22603 Hamburg, Germany

In an application of the combination of microfluidics with in-situ GISAXS (grazing incidence small angle x-ray scattering) we investigate the early stages of the attachment of gold nanoparticles to polyelectrolyte layers. The study clearly shows the differing kinetics of the surface coverage of slightly negatively charged nanoparticles onto negatively charged layers of polystyrene sulfonate (PSS) and positively charged polyallylamine hydrochloride (PAH), respectively. With the microfocussed beam of a highly brilliant x-ray third generation synchrotron a high time resolution is achieved. The microfluidic investigation with a special designed cell [1] is accompanied by GISAXS dip coating experiments [2] also performed in-situ.

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

[2] J. Perlich et al., *Phys. Status Solidi RRL* 6, 253 (2012).

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

CPP 34.23 Wed 16:30 Poster C

Oscillations and Avalanches in Two-Dimensional Flowing Crystals — ●JEAN-BAPTISTE FLEURY¹, OHLE CAUSSEN², STEPHAN HERMINGHAUS², MARTIN BRINKMANN², and RALF SEEMANN^{1,2} — ¹Experimental Physics, University of Saarland, Saarbrücken, Germany — ²Max-Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

We study the mechanical response and the stability of monodisperse droplet packings in quasi 2d micro-channels under longitudinal compression. Depending on the exact choice of parameter a static droplet arrangement can be mechanically unstable and segregate into domains of higher and lower packing fraction. When these droplet arrangements with negative compressibility slowly flow along a microfluidic channel periodic density oscillations between the stable droplet packings can be found. For increasing flow velocity the sections of larger and lower packing fraction increase, finally leading to complex non-equilibrium droplet re-arrangements similar to avalanches. We will experimentally and theoretically discuss the mechanisms of the dynamical droplet re-arrangements in an out-of-equilibrium microfluidic system.

CPP 35: Poster: Biomaterials and Biopolymers (joint session BP/CPP)

Time: Wednesday 16:30–18:30

Location: Poster C

CPP 35.1 Wed 16:30 Poster C

Structur formation of a coarse-grained bead model — ●BENNO WERLICH¹, MARK TAYLOR², and WOLFGANG PAUL¹ — ¹Institut für Physik, Martin-Luther University Halle-Wittenberg, Halle(Saale), Germany — ²Department of Physics, Hiram College, Ohio, USA

We study structure formation of single stiff, coarse-grained hard-sphere chains by means of Wang-Landau type Monte Carlo simulations. Stiffness is introduced by allowing a varying degree of overlap of bonded hard spheres. Collapse of these chains is introduced by a square-well attraction between non-bonded spheres. Depending on the degree of stiffness different, non-trivial morphologies like, e.g., helical structures, occur in the collapsed state. The transitions between different states are determined by an analysis of thermodynamic response functions. For the simulations we implemented the so-called Stochastic Approximation Monte Carlo method which has the advantage of implementing a very general and simple iteration scheme.

CPP 35.2 Wed 16:30 Poster C

Nano-Mechanics of Type I Collagen Fibrils in Aqueous Solution — ●DIANA VOIGT, JULIA HANN, EIKE-CHRISTIAN SPITZNER, and ROBERT MAGERLE — Chemnitz University of Technologie, Institut of Physics, Germany

We investigate purified type I collagen extracted from bovine hide. In aqueous solution, triple helices of collagen molecules (tropocollagens) form fibrils driven by hydrogen bonding processes. Single collagen fibrils, deposited on a silicon substrate, were exposed to an aqueous solution with controlled pH and salt concentration. We use in-situ multi-setpoint intermittent contact mode (MUSIC-Mode) atomic force microscopy for quantitative imaging of collagen fibrils and their me-

chanical properties in aqueous solution. Furthermore we control the electrochemical potential between the sample and the AFM probe.

CPP 35.3 Wed 16:30 Poster C

Ab-initio molecular dynamics of photoacids in aqueous environment — ●GÜL BEKÇIOĞLU, CHRISTOPH ALLOLIO, and DANIEL SEBASTIANI — Institute of Chemistry, Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 4, 06120 Halle (Saale)

Biophysical processes often take place based on proton relay along a hydrogen bonded chain.[1] Such proton transfer reactions along "water wires" are difficult to observe directly inside a protein. Photosensitive acid/base systems provide a method to control and study ultrafast proton transport via infrared spectroscopy.[2] Hydroxyquinolines (HQ) are simultaneously photoacids and photobases. Departing from our successful simulation of the excited state dynamics and fluorescence shift of the related N-methyl-6-quinolone [3], we study the ground and excited state solvation of different HQs, focussing on the identification of water wires and excited state protonation dynamics.

[1] H. Luecke, H.-T. Richter, J. K. Lanyi, *Science* **280** (1998), 1934.

[2] O. F. Mohammed, D. Pines, J. Dreyer, E. Pines and E. T. J. Nibbering., *Science* **310** (2005), 5745.

[3] C. Allolio, M. Sajadi, N. P. Ernsting and D. Sebastiani, *Angew. Chem. Int. Ed.* accepted, (2012).

CPP 35.4 Wed 16:30 Poster C

Water absorption of cellulose fibers and possible morphological influences — ●PATRICE KREIML^{1,2}, CHRISTIAN GANSER^{1,2}, ROLAND MORAK¹, OSKAR PARIS¹, ROBERT SCHENNACH^{2,3}, and CHRISTIAN TEICHERT^{1,2} — ¹Institute of Physics, Montanuniversität Leoben, Franz Josef - Str. 18, 8700 Leoben, Austria — ²Christian

Doppler Laboratory for Surface Chemical and Physical Fundamentals of Paper Strength, Graz University of Technology, Petersgasse 16/2, 8010 Graz, Austria — ³Institute of Solid State Physics, Graz University of Technology, Petersgasse 16/2, 8010 Graz, Austria

Fibers are used in textiles, hygiene products, and medical applications. The water absorption is an important property in the applications mentioned. In this study, the water absorption of different fiber types was measured. The method of choice is a micro balance, which allows to detect a change in mass by increasing and decreasing the partial water vapor pressure at a constant temperature. The result is an isothermal hysteresis that yields the water absorption and desorption with respect to the relative humidity. Additionally, the morphology of two sets of viscose fibers was characterized by atomic-force microscopy (AFM). The two sets of samples were produced under the same conditions, but exhibited a difference in water absorption. A comprehensive roughness analysis showed no significant differences in the roughness parameters. However, on the surfaces of all samples trenches could be observed. Preliminary results indicate an influence of trench density on the water absorption. Supported by Kelheim Fibres and the Christian Doppler Research Society, Vienna Austria.

CPP 35.5 Wed 16:30 Poster C

Hierarchical Multi-Step Folding of Polymer Bilayers —

•GEORGI STOYCHEV^{1,2}, SEBASTIAN TURCAUD³, JOHN DUNLOP³, and LEONID IONOV¹ — ¹Leibniz Institute of Polymer Research Dresden, Hohestr. 6, 01069, Dresden, Germany — ²Technische Universität Dresden, Physical Chemistry of Polymer Materials, 01062, Dresden, Germany — ³Am Mühlenberg 1, 14424, Potsdam, Germany

We investigated the actuation of patterned bilayers placed on a substrate. We found that films display several kinds of actuation behavior such as wrinkling, bending and folding that result in a variety of shapes. Based on experiments and modeling, we argued that rectangular bilayers start to roll from the corners due to quicker diffusion of water. Rolling from long-side starts later and dominates at high aspect ratio[1].

It was also demonstrated that one can introduce hinges into the folded structure by proper design of the bilayers external shape without having to use site selective deposition of active polymers. Experimental observations lead us to derive four empirical rules backed up by theoretical understanding as well as simulations. We then demonstrated how those rules can be used to direct the folding of edge-activated polymer bilayers through a concrete example - the design of a 3D pyramid[2].

[1] Stoychev et al, "Hierarchical Multi-Step Folding of Polymer Bilayers", *Adv.Func.Mat.*, published online Nov 26, 2012

[2] Stoychev et al, "Shape-Programmed Folding of Stimuli-Responsive Polymer Bilayers", *ACS Nano*, 2012, 6(5), 3925-3934

CPP 36: Poster: (Hydro)gels and Elastomers

Time: Wednesday 16:30–18:30

Location: Poster C

CPP 36.1 Wed 16:30 Poster C

The distribution of segmental order in polymer networks — •MICHAEL LANG¹ and JENS-UWE SOMMER^{1,2} — ¹Leibniz Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden — ²Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden

We discuss the distribution function of the segment orientation order parameter in entangled networks. The distribution function is derived from a tube model of polymer entanglements assuming random walk statistics of the tube. Monomer fluctuations along the tube are assumed to follow the phantom model as shown in a previous work [M. Lang, J.-U. Sommer, *Physical Review Letters* 104 (2010) 177801]. The predictions are compared with simulation data of model networks that were created using the bond fluctuation method. The comparison reveals that local fluctuations of the tube statistics do not affect the distribution function as averaged over the full sample. Instead, length fluctuations of the confining tube control the shape of the distribution function. Furthermore, a narrowing of the distribution function is determined, if the cross-linking occurs on the time scale of the relaxation of the network strands. Almost instantaneously cross-linked polydisperse samples do not show this narrowing and are well described by tube length fluctuations that agree to previous work on the dynamics of melts of star polymers.

CPP 36.2 Wed 16:30 Poster C

Poly(N-isopropylacrylamide) chains adsorbed on silica nanoparticles: A dielectric study of the phase transition of interfacial pNIPAM — •MARIEKE FÜLLBRANDT^{1,2}, SARAH T. TURNER¹, REGINE VON KLITZING¹, and ANDREAS SCHÖNHALS² — ¹Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Strasse des 17. Juni 124, D-10623 Berlin — ²BAM Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, D-12205 Berlin

Poly(N-isopropylacrylamide)(pNIPAM) is adsorbed on silica nanoparticles. In bulk phase linear pNIPAM shows a lower critical solution temperature (LCST) at about 32°C. In general the physical properties of constrained polymers differ from those of the bulk phase. Adsorbed pNIPAM on surfaces can have interesting applications in functionalized interfaces with thermosensitive properties. Such applications require fundamental knowledge of the transition behaviour and mobility of adsorbed pNIPAM chains.

Dielectric Relaxation Spectroscopy (DRS) is applied in a frequency range of 10⁻¹ to 10⁶ Hz. By using charges as probes the phase transition of pNIPAM can be monitored by both the temperature dependence of the DC conductivity and the frequency dependence of the complex conductivity spectra [1]. The formation of a Si/pNIPAM

core/shell particle where charges are trapped/ blocked at the interface evokes a Maxwell/Wagner/Sillars polarization. For structural information DLS measurements and TEM images are added. [1] M. Füllbrandt, R. von Klitzing and A. Schönhals, *Soft Matter*, 2012, 8, 12116-12123.

CPP 36.3 Wed 16:30 Poster C

Kinetics of aggregation in micellar solutions of thermoresponsive triblock copolymers: influence of concentration, start and target temperature — JOSEPH ADELSBERGER¹, AMIT KULKARNI¹, ISABELLE GRILLO², MELISSA SHARP³, ACHILLE M. BIVIGOU-KOUMBA⁴, ANDRÉ LASCHEWSKY⁴, PETER MÜLER-BUSCHBAUM¹, and •CHRISTINE M. PAPADAKIS¹ — ¹TU München, Physik-Department, Physik weicher Materie, Garching — ²Institut Laue-Langevin, Grenoble, France — ³European Spallation Source, Lund, Sweden — ⁴Uni Potsdam, Institut für Chemie, Potsdam-Golm

Micellar solutions of thermoresponsive block copolymers respond to a small change of temperature across the cloud point with a strong volume change. We have investigated triblock copolymers having a long poly(N-isopropylacrylamide) (PNIPAM) middle block and two short polystyrene (PS) end blocks. Temperature-resolved SANS with contrast matching revealed the collapse of the micellar shell and the subsequent aggregation [1]. Time-resolved SANS during a temperature jump showed that the process involves a number of steps, such as the formation of small imperfect aggregates, their densification and their growth by attachment of single micelles and finally by coagulation [2]. The time constants depend on polymer concentration, start and target temperature [2].

1. J. Adelsberger, C.M. Papadakis et al., *Macromolecules* **43**, 2490 (2010) and *Colloid Polym. Sci.* **289**, 711 (2011).

2. J. Adelsberger, C.M. Papadakis et al., *Macromol. Rapid Commun.* **33**, 254 (2012) and *Soft Matter*, DOI:10.1039/C2SM27152D

CPP 36.4 Wed 16:30 Poster C

Rheological characterization of PDMS-based magnetoelastomers — •RUDOLF HASSLACHER¹, VITOR C. BARROSO¹, FRANZ HIPTMAIR², ZOLTAN MAJOR², KERSTIN SCHINDLER³, CHRISTIAN WOLFRUM³, and SABINE HILD¹ — ¹Institute of Polymer Science, Johannes Kepler University of Linz, Altenberger Strasse 69, 4040 Linz, Austria — ²Institute of Polymer Product Engineering, Johannes Kepler University of Linz, Altenberger Strasse 69, 4040 Linz, Austria — ³Eckart GmbH, Guentersthal 4, 91235 Hartenstein, Germany

Magnetoelastomers are hybrid materials based on elastomers and magnetic particles. Due to their magnetic features, their mechanical properties and shape can be controlled by external magnetic fields. Applications as mechanical actuators, mechanical dampers or for vibration

reduction are conceivable.

Depending on the particle material, size and their distribution and arrangement inside the cured elastomeric matrix, the obtained mechanical properties (and possible applications) can be varied. Ultimately the movement of the particles is heavily dependent on the viscosity of the whole composite.

During this work, the preparation of the magnetoelastomeric material and corresponding rheological characterisation were carried out. The isotropic materials consisted of a crosslinkable polydimethylsiloxane (PDMS) matrix filled with different iron particles (distinguishable by shape and functionalities). The aim is to study the crosslinking behaviour and its dependence on the particle characteristics by means of time resolved rheological measurements.

CPP 36.5 Wed 16:30 Poster C

Wetting induced structure formation in elastic porous media — ●ZRINKA GATTIN, OHLE CLAUSSEN, STEPHAN HERMINGHAUS, and MARTIN BRINKMANN — MPI DS, Am Fassberg 17, 37077 Gottingen, Germany

The interplay between the elasticity of a porous matrix and interfacial stresses can give rise to a wide variety of unexpected phenomena including spontaneous symmetry breaking and pattern formation.

Many properties of a fibre network undergo large changes when exposed to a wetting liquid. The mechanical response of an elastic fibre network, for example, to compression or shear changes noticeably between the dry and the wet state. A number of processes can lead to the formation of liquid domains in a fibre network. This includes phase separation of the ambient fluid, impact of aerosol droplets on fibres, or spontaneous imbibitions of liquid. In all of these cases the elasticity of the elastic matrix in combination with its wetting properties will have an effect on the dynamics of these processes.

Motivated by experiments on the demixing of binary liquids in polymer gels we study the formation and interaction of liquid droplets in a dilute elastic medium. To model the phase separating liquids we use a lattice gas model while the elastic matrix is represented by a network of tethered particles which are interacting with the fluid phases. Here, we present preliminary results on the deformation of the network due to interfacial stresses for different configurations of the liquid domains after demixing. The results of our simulations are compared to predictions of a simple continuum model of the elastic matrix.

CPP 36.6 Wed 16:30 Poster C

Dielectric strength and electro-mechanical instability in soft insulating elastomers — ●STEFAN BEST, MATTHIAS KOLLOSCHKE, and REIMUND GERHARD — ACMP, Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht-Str. 24/25, 14476 Potsdam-Golm, Germany

The dielectric breakdown strength of polymer materials is of particular interest for many technological applications such as cable insulation, polymer capacitors and emerging systems that rely on soft polymers, such as energy harvesting or voltage tunable optics. We present experimental strategies to assess the impact of material properties and preparation methods on the dielectric breakdown strength of soft insulating polymers. This is studied on un-stretched Elastomers of various material stiffnesses, which can be varied through the preparation methods. Also, the breakdown strength was measured as a function of stretch ratio. The breakdown strength of un-stretched elastomers was found to increase with material stiffness, since breakdown occurs due to an electro-mechanical instability mechanism. Relatively higher break-

down strength was observed on pre-stretched, clamped elastomers. It is found, that very high pre-stretch prevents the electro-mechanical instability such that dielectric breakdown strength becomes independent of stretch ratio and thus the true material breakdown strength is observed. The results are found to compare well with theories in literature.

CPP 36.7 Wed 16:30 Poster C

About the elastic nature of the demixing transition of aqueous PNIPAM solutions — ●MARTINE PHILIPP¹, ULRICH MÜLLER², RALITSA ALEKSANDROVA², ROLAND SANCTUARY², PETER MÜLLER-BUSCHBAUM¹, and JAN K. KRÜGER² — ¹TU München, Physik-Department, LS Funktionelle Materialien, Garching, Germany — ²Université du Luxembourg, LPM, Luxembourg, Luxembourg

The demixing transition of aqueous solutions of poly(N-isopropylacrylamide) (PNIPAM) has been widely investigated in basic and applied research. It is of the lower critical solution temperature type. Due to the large volume change accompanying this phase separation, it is denoted as a volume transition. Only few experiments were dedicated to the elastic properties at this transition. However, one hint exists that the longitudinal elastic modulus may be its inverse order parameter susceptibility [1]. Here we discuss the competitive behaviour of mass density and the longitudinal elastic modulus across the demixing transition in dependence of temperature and PNIPAM concentration [2]. Brillouin spectroscopy indeed proves the governing role of the longitudinal elastic modulus for this phase separation mechanism. Moreover, Brillouin spectra recorded across the phase transition allow following the growth of PNIPAM-rich agglomerates with gel-like mechanical consistency embedded in the liquid PNIPAM-poor phase. This result clearly disproves the widespread opinion that the demixed PNIPAM-rich agglomerates are glassy.

[1] S. Hirotsu, Phase Transitions 47, 183 (1994) [2] M. Philipp, U. Müller, R. Aleksandrova et al., Soft Matter 8, 11387 (2012)

CPP 36.8 Wed 16:30 Poster C

Co-non-solvency effect of adsorbed thermo-responsive gel particles — ●MARCEL RICHTER, MELANIE HUNNENMÖRDER, and REGINE VON KLITZING — TU Berlin

During the last decades microgels made of N-isopropylacrylamide (PNIPAM) have attracted much interest and were studied by several techniques like atomic force microscopy (AFM) and dynamic light scattering (DLS) [1]. These polymer particles show thermo responsive behaviour and can therefore be classified as *smart* materials. The Co-non-solvency effect in the different water/ solvent compositions are well investigated for the bulk phase [2, 3] but not at the surface. Those colloidal particles are of great interest as carrier systems and sensors [4]. For this purpose the understanding of such particles in different organic solvent mixtures is necessary. The presented study focuses on the swelling behaviour of PNIPAM and PNIPAM-co-AAA microgels in different water/ solvent compositions. The question will be answered: How much the particles swell from the dry to the liquid state? Furthermore, the particle size in different water/ solvent ratio is investigated. The used solvents are ethanol, iso-propanol and tetrahydrofuran. The size of microgels is determined by Dynamic Light Scattering and Scanning Force Microscopy. [1] K. Kratz, T. Hellweg, W. Eimer, Polymer (2001), 42, 6531 [2] B. Saunders et al, Macromolecules (1997), 30, 482 [3] Christine Scherzinger et al, Macromolecules (2010), 43, 6829 [4] J. Kim, Angewandte Chemie (2005), 117, 1357

CPP 37: Poster: Focus: Van der Waals at soft matter interfaces: structure and dynamics

Time: Wednesday 16:30–18:30

Location: Poster C

CPP 37.1 Wed 16:30 Poster C

Structure and Dynamics in Frustrated Liquid Crystal Films Influenced by Subsurface Substrate Material — ●KATHRIN RADSCHKEIT, DANIELA TÄUBER, and CHRISTIAN VON BORCZYKOWSKI — nanoMA, TU-Chemnitz, Institut für Physik

Liquid crystals are known to be very sensitive to chemical and topological properties of confining interfaces. Recently we found an influence of the subsurface substrate composition on the structure in thin frustrated 8CB liquid crystal films on Si with native or 100 nm thermal oxide [1]. Observation in polarization resolved reflected light during

heating from the smectic A to the nematic phase and subsequent cooling, reveals different timescales of the phase transition of thin 8CB films on the two types of substrate. We ascribe the observed differences to van der Waals interactions with the underlying silicon in case of the native oxide, whereas the thermal oxide suffices to shield those interactions. Additional information about the dynamics in thin liquid crystal films is obtained from correlations of s- and p-polarization resolved fluorescence intensities from diffusing tracer molecules, extending previous studies in unpolarized light [2].

[1] B. Schulz, D. Täuber, J. Schuster, T. Baumgärtel and C. von Borczykowski, Soft Matter 7 (2011) 7431. [2] B. Schulz, D. Täuber,

F. Friedriszik, H. Graaf, J. Schuster and C. von Borczyskowski, PCCP 12 (2010) 11555.

CPP 37.2 Wed 16:30 Poster C

Bimodal MUSIC Mode Atomic Force Microscopy on Polymers — ●EIKE-CHRISTIAN SPITZNER¹, CHRISTIAN DIETZ², and ROBERT MAGERLE¹ — ¹Chemische Physik, TU Chemnitz, D-09107 Chemnitz — ²Center of Smart Interfaces, TU Darmstadt, D-64287 Darmstadt

Multi-set point intermittent contact (MUSIC) mode atomic force microscopy (AFM) is based on point wise recording amplitude and phase of an AFM cantilever as the tip sample distance is reduced (APD

curves). The technique emulates intermittent contact mode AFM without a feedback loop that causes artifacts in height and phase images. Here, we demonstrate multifrequency MUSIC mode AFM by simultaneous excitation of the first two eigenmodes of the cantilever. Furthermore, the frequency of the first eigenmode is kept at resonance during approach to prevent damping of the amplitude caused by attractive interactions. Thus, the attractive regime in the APD curves is suppressed. This enables a straight forward calculation of the tip indentation also on surfaces that exhibit strong attractive interactions between tip and sample. We show results for collagen fibrils in bovine tendon as well as other polymeric surfaces. Furthermore, enhanced contrast in the phase images of the second eigenmode is demonstrated.

CPP 38: SYMM: Computational Challenges in Scale-Bridging Modeling of Materials

Time: Thursday 9:30–12:00

Location: H1

Invited Talk

CPP 38.1 Thu 9:30 H1

Challenges for first-principles based computation of properties of oxide materials — ●KARSTEN ALBE — TU Darmstadt, FB 11, FG Materialmodellierung, Petersenstr. 32, D-64287 Darmstadt

Calculations based on density functional theory (DFT) have been the mainstay of theoretical studies of the properties of semiconductor and oxide materials over the past few decades. Despite of their significant successes, challenges remain in adapting these methods for predictive simulations that are quantitatively useful in predicting complex device properties. Increasing computing power and improved theoretical methods taking advantage of ever more powerful computer hardware offer the possibility that computational modelling may finally allow a virtual materials design by truly predictive simulations. In this contribution, I will give examples for successes and failures in calculating bulk, point defect and surface properties of transparent conducting as well as ferroelectric oxides and describe the remaining challenges.

Invited Talk

CPP 38.2 Thu 10:00 H1

Deformation and Fracture of Solids: Tough Nuts at Atomic and Continuum Scales — ●PETER GUMBSCH^{1,2}, MATOUS MROVEC^{1,2}, KINSHUK SRIVASTAVA¹, and DANIEL WEYGAND¹ — ¹Institut für Applied Materials IAM, Karlsruhe Institute of Technology KIT — ²Fraunhofer IWM, Freiburg

Multiscale modeling of deformation processes in crystalline materials poses several challenges although the basic physical process, the motion of dislocations, is well understood. I will use the deformation of single crystalline alpha-iron to illustrate these challenges.

To feed dislocation dynamics with realistic atomistic information requires a reliable and computationally efficient description of the atomic interactions. We use a recently developed magnetic bond-order potential (BOP). Dislocation mobility laws for discrete dislocation dynamics (DDD) studies of large dislocation ensembles then require consideration of the full local stress state in a mesoscopic mobility law since it turned out that the effect of non-glide stresses and orientation of the applied loading is crucial for capturing the non-Schmid behavior.

Averaging the behavior of discrete dislocations into continuum mechanical equations is even more difficult. It requires a homogenization of the dislocation fields including a description of their multiplication and mutual interaction. The mathematical framework for such a continuum field theory is still not available. I will present a kinematically consistent continuum description of the dynamics of curved dislocation systems as a first approach to such a continuum field theory.

Invited Talk

CPP 38.3 Thu 10:30 H1

Crucial Issues and Future Directions of Through-Process Modeling — ●GUENTER GOTTSTEIN — RWTH Aachen University, Institut of Physical Metallurgy and Metal Physics, Aachen, Germany

Computer simulation of materials processing and properties has advanced to an established field and indispensable research topic in materials science and engineering during the past decade. Moreover, it has grown to a powerful and accepted tool for commercial alloy and process development. While the general theory has been laid out, physics based scale-bridging modeling approaches have been developed and are currently employed also in industrial environments, flexible in-

terfacing has become available and automated simulation is currently being tested, there are still bottlenecks that impede the ease of application and the predictive power of these tools and urgently need to be addressed. Such needs include reliable experimental databases, the bridging of knowledge gaps on critical phenomena like nucleation, interacting microstructural evolution processes that require vastly different computation times, inverse modeling algorithms etc. Finally, despite of the remarkable advances in available computer power, computer simulation still suffers from too low computational speed to address statistically significant system sizes and to lend itself to process control. More recent concepts will be introduced, in particular in view of the changing philosophy of computer architecture and the increasing availability of massively parallel computing power, which may actually require a departure from conventional and established modeling concepts.

Invited Talk

CPP 38.4 Thu 11:00 H1

Adaptive Resolution Simulations for Soft Matter: Applications and New Developments — ●KURT KREMER — Max Planck Institute for Polymer Research

The relation between atomistic structure, architecture, molecular weight and material properties is a basic concern of modern soft matter science. A typical additional focus is on surface and interface aspects or the relation between structure and function in nanoscopic molecular assemblies. Here computer simulations on different levels of resolution play an increasingly important role. To progress further, adaptive schemes are being developed, which allow for a free exchange of particles (atoms, molecules) between the different levels of resolution. The lecture will concentrate on these methods to couple particle based simulations to continuum as well as to include quantum effects will be presented. Furthermore the extension to open systems MD as well as new recent methodology advances will be explained. A general review on the first part can be found in M. Praprotnik, L. Delle Site, and K. Kremer, *Ann. Rev. Phys. Chem.* 59, (2008) and recent advances in S. Fritsch et al. *Phys. Rev. Lett.* 108, 170602 (2012)

Invited Talk

CPP 38.5 Thu 11:30 H1

Materials by design — ●MARKUS BUEHLER — MIT, 77 Mass. Ave, Cambridge, MA 02139

Biological materials are synthesized, controlled and used for an astonishing variety of purposes including structural support, force generation, mass transport, catalysis, or energy conversion. By incorporating concepts from biology and engineering, computational modeling has led the way in identifying the core principles that link the molecular structure of biomaterials at scales of nanometers to physiological scales at the level of tissues. The use of the world's fastest supercomputers allows us to predict properties of complex materials from first principles, realized in a multiscale modeling approach that spans massive ranges in scale. Combined with experimental studies, such in silico models allow us to simulate disease, understand catastrophic failure of tissues, and enable us to translate concepts from the living world into material designs that blur the distinction between the living and non-living systems. We discuss challenges and opportunities in new methods of scale bridging.

CPP 39: Organic Electronics and Photovoltaics IV (joint session CPP/HL/O/DS)

Time: Thursday 9:30–13:00

Location: H34

Invited Talk

CPP 39.1 Thu 9:30 H34

Influence of morphology on organic solar cell performance comparing crystalline diindenoperylene (DIP) and its amorphous derivative tetraphenylidibenzoperiflanthene (DBP) — STEFAN GROB, MARK GRUBER, ULRICH HÖRMANN, and WOLFGANG BRÜTTING — Institute of Physics, University of Augsburg, Germany

The DIP molecule, consisting of seven benzene and two cyclopentadiene rings, forms the backbone of the DBP molecule, which has two further benzene rings and four additional, rotatable phenyl groups. Compared to the planar arrangement of DIP, the four phenyl groups give DBP a more three-dimensional shape, changing the growth behavior in thin films completely. While we observe crystalline domains of almost upright standing DIP, layers of DBP exhibit an amorphous character and therefore a relatively small exciton diffusion length, being about ten times shorter than that of its crystalline counterpart. However, the drawback of the upright standing arrangement of DIP molecules is the unfavorable orientation of the transition dipole moment resulting in a low absorption coefficient. In contrast, the structural disorder in DBP combined with a little smaller optical gap leads to light absorption which is about eight times higher than in DIP, whereby the short-circuit current density almost doubles in corresponding solar cell devices. Moreover, open circuit voltages are high and - due to similar energy level alignments - comparable, by using the materials both as donor with C60 (0.9 V) and as acceptor with 6T (1.2 V). Based on these results, we discuss the influence of different film structure and morphology on electrical transport and device performance.

CPP 39.2 Thu 10:00 H34

Influence of fluorine content in manipulating the nanomorphology of PTB7:PC70BM bulk heterojunction systems — SHUAI GUO¹, JING NING¹, VOLKER KÖRSTGENS¹, YUAN YAO¹, CHEN LIN¹, STEPHAN ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany — ²HASYLAB at DESY, 22603 Hamburg, Germany

Polymer-based photovoltaics have drawn tremendous attention in both basic research and application fields during the last decade. Here, the up-to-date highest efficient bulk heterojunction system PTB7 with varied fluorine content and the fullerene derivative PC70BM are thoroughly investigated. It is known that the amount of fluorine along the polymer chain strongly influences the film formation and therefore the solar cell performance. Additionally, it is of great interest to explore the effect of solvent additive 1,8-diiodooctane (DIO) on differently fluorinated films. To address the relation between the morphology and efficiency completely, a series of measurements have been done. The film surface structure is investigated by optical microscopy and AFM. The inner film structures, crystal orientation as well as the crystallinity are probed by advanced scattering techniques such as XRR, GISAXS and GIWAXS. By integrating all data, the three-dimensional morphology of the active layer is detected. Consequently, the different morphologies introduced by varying the fluorine content and the addition of DIO are determined and compared with the corresponding performance of these systems.

CPP 39.3 Thu 10:15 H34

Influence of nanostructural changes on the charge carrier dynamics in PTB7 based solar cells — ANDREAS ZUSAN¹, ANDREAS BAUMANN², JENS LORRMANN¹, CARSTEN DEIBEL¹, and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — ²Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg

For organic bulk heterojunction solar cells, the blend morphology is one of the most crucial parameters influencing the device performance. Inducing nanostructural changes by means of the use of processing additives is a common practice to increase the power conversion efficiency. Hence, understanding the effect of modified structural properties of organic layers on the charge carrier transport and lifetime is a key issue for further progress in organic photovoltaics. In this context, we applied our novel charge extraction technique OTRACE (Open Circuit Corrected Transient Charge Extraction) to high efficiency solar cells made from the low-bandgap polymer PTB7 in combination with PC70BM using the solvent additive diiodooctane (DIO). The results

show two different nongeminate decay regimes identified as a fast direct recombination of free polarons and a trap assisted decay. We find that the DIO induced alteration of the morphology significantly reduces the recombination order of the first regime, whereas it has no influence on the second part arising from the delayed emission of trapped charges. Our explanation based on a multiple-trapping-and-release approach clarifies the large impact of phase separation on charge carrier dynamics.

CPP 39.4 Thu 10:30 H34

Diffusion limited charge generation from fullerene excitons in low bandgap polymer solar cells — CLARE DYER-SMITH, IAN HOWARD, and FRÉDÉRIC LAQUAI — Max Planck Institut für Polymerforschung, Mainz, Germany

Organic solar cells with high power conversion efficiencies have been realised in recent years by the use of low bandgap polymers in combination with C70-based electron acceptors to provide good absorption coverage across the entire solar emission spectrum. Diffusion-limited charge generation from fullerene excitons has been observed in such blends, including the high-performance PTB7:PC70BM blend system which is the subject of the present study. We characterise the diffusion-limited charge generation from fullerene excitons in this system using transient absorption and photoluminescence spectroscopy. Fitting to a simple exciton quenching model allows us to determine the size of fullerene domains in the blend, showing quantitatively how blend morphology limits device performance, and allowing us to identify selection criteria for the optimum blend morphology in devices based upon light-absorbing fullerene acceptors.

CPP 39.5 Thu 10:45 H34

Impact of molecular weight on the intrinsic charge carrier mobility of Si-PCPDTBT:[C70]PCBM thin films — ANDREAS FRITZE¹, ANDREAS SPERLICH¹, ANDREAS ZUSAN¹, CARSTEN DEIBEL¹, and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²ZAE Bayern, 97074 Würzburg

We investigated the influence of the molecular weight on the performance of solar cells from solution processed Si-PCPDTBT:[C70]PCBM blends. A significant increase in the short circuit current density j_{SC} was found with increasing molecular weight of the polymer. To explain this behavior, we performed transient microwave conductivity (TRMC) experiments and found much higher intrinsic mobilities in thin films based on the higher molecular weight donor. In order to distinguish between the influence of intra- and intermolecular charge transport on the obtained intrinsic TRMC mobility, we used two different solvents to influence the molecular environment in the film. We discuss our findings in view of the impact of the local order, influenced by the molecular weight on the performance of organic solar cells.

CPP 39.6 Thu 11:00 H34

Charge generation and recombination in PCPDTBT:PCBM and PSBTBT:PCBM bulk heterojunction photovoltaic blends — FABIAN ETZOLD, IAN HOWARD, MICHAEL MEISTER, and FRÉDÉRIC LAQUAI — Max Planck Research Group for Organic Optoelectronics, Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

We present a comparative study of the photophysical processes leading to photocurrent generation and photocurrent loss in photovoltaic blends of the low-bandgap polymer PCPDTBT with PCBM and its silicon-substituted analogue PSBTBT with PCBM studied by Vis-NIR transient absorption pump-probe spectroscopy and variable time-delay double-pump photocurrent extraction experiments. Our experiments demonstrate that the power conversion efficiency of PCPDTBT:PCBM blends is largely limited by sub-nanosecond geminate recombination of interfacial charge-transfer states plus fast non-geminate recombination of free charges competing efficiently with charge extraction. In comparison photovoltaic blends of the silicon-substituted polymer PSBTBT with PCBM exhibit significantly less geminate recombination in conjunction with much slower non-geminate recombination of free charges leading in turn to substantially higher photocurrents and fill factors and thus overall increased photovoltaic performance. We also observed a pronounced excitation wavelength dependence of the pho-

tophysical processes occurring after excitation of either the polymer or the fullerene component of the blend at different photon energies. [1] F. Etzold et al., *J. Am. Chem. Soc.* 2012, 134 (25), 10569-10583.

15 min. break

CPP 39.7 Thu 11:30 H34

Charge Generation in PBDTPD:PCBM and Si-PCPDTBT:PCBM Solar Cells: The Influence of Excess Photon Energy and Electronic Energy Level Offsets — ●STEVE ALBRECHT¹, KOEN VANDEWAL², ALBERTO SALLEO², and DIETER NEHER¹ — ¹University of Potsdam, Soft Matter Physics, Potsdam, Germany — ²Stanford University, Department of Materials Science and Engineering, Stanford, USA

In the last years a dramatic increase in organic solar cell efficiency has been reported with polymers and fullerene derivatives processed from solution. However, the fundamental process involved in the conversion of absorbed photons to free charges is still not fully understood. In this work, we use time delayed collection field (TDCF) [1] with variable excitation wavelength to gain insight into the effect of the excess photon energy on the quantum efficiency and field-dependence of free charge carrier generation. With two high efficiency model systems showing either field independent CT-state splitting (PBDTPD:PCBM) or a weak field-dependence of free charge formation (Si-PCPDTBT:PCBM), we show how the field-dependence changes with direct CT state excitation in the absorption region below the band-gap. Additionally, we show how generation and bimolecular recombination is affected when the fullerene derivative PCBM is exchanged by higher LUMO adducts ICMA, ICBA or ICTA with reduced driving force for CT-state splitting.

[1] Albrecht, S.; Janietz, S.; Schindler, W.; Frisch, J.; Neher, D., *Journal of the American Chemical Society* 134 (36), 14932 (2012).

CPP 39.8 Thu 11:45 H34

Sub-Bandgap Absorption in Polythiophene–Fullerene Heterojunctions: Experiment and Theory — ●WICHARD BEENKEN, FELIX HERRMANN, MARTIN PRESSELT, HARALD HOPPE, SVIATOSLAV SHOKHOVETS, GERHARD GOBSCH, and ERICH RUNGE — Technische Universität Ilmenau, Institut für Physik and Institut für Mikro- und Nanotechnologien, 98693 Ilmenau, Germany

Most high-performance organic solar cells base on P3HT/PCBM bulk-heterojunctions. Spectroscopy of the sub-bandgap region, i.e., below the bulk absorption of the individual components, provides unique opportunities to study interface-related properties. In order to characterize some of the unsettled spectral features, we applied quantum-chemical calculations of a oligothiophene–fullerene model complex, which in particular allow us to identify spectral signatures of charge-transfer excitons in the sub-bandgap absorption and external quantum efficiency.

CPP 39.9 Thu 12:00 H34

A new multiscale modeling method for simulating the loss processes in polymer solar cell nanodevices — ●ANTON PERSHIN, SERGI DONETS, and STEPHAN A. BAEURLE — Institute of Physical and Theoretical Chemistry, University of Regensburg, D-93040 Regensburg, Germany

The photoelectric power conversion efficiency of polymer solar cells is till now, compared to conventional inorganic solar cells, relatively low with maximum values ranging from 7% to 8%. This essentially relates to the existence of exciton and charge carrier loss phenomena, significantly reducing the performance of polymer solar cells. Here, we introduce a new computer simulation technique [1], which permits to explore the causes for the occurrence of such phenomena at the nanoscale and to design new photovoltaic materials with optimized opto-electronic properties. Using our approach, we find that the disjunction of continuous percolation paths leads to the creation of dead ends, resulting in charge carrier losses through charge recom-

bination. Moreover, we observe that defects are characterized by a low exciton dissociation efficiency due to a high charge accumulation, counteracting the charge generation process. Finally, by analyzing the photovoltaic behavior of the nanostructures under different circuit conditions, we demonstrate that charge injection at the electrodes determines the impact of the defects on the solar cell performance. [1] A. Pershin, S. Donets, S.A. Baeurle, *J. Chem. Phys.* 136, 194102 (2012).

CPP 39.10 Thu 12:15 H34

Morphology and Charge Transport in Polythiophene/PCBM Blends: Insight from Molecular Simulations — ●OLGA GUSKOVA¹, JULIA ROMANOVA², ANDREAS JOHN¹, PETER FRIEDEL¹, and JENS-UWE SOMMER^{1,3} — ¹Leibniz Institute of Polymer Research, Dresden, Germany — ²University of Namur, Namur, Belgium — ³TU Dresden, Dresden, Germany

Combined structural-computational approach to study the organic photovoltaic materials, namely mixtures of polythiophenes (donor, D) and [6,6]phenyl-C61-butyric acid methyl ester (acceptor, A) was applied. The quantum mechanical computational level was used (1) to improve the force field for subsequent molecular dynamics (MD) modeling, (2) to calculate the ionization energies, electron affinities, HOMO/LUMO energies and charge transfer characteristics of D/A pair. We have performed a large-scale all-atomistic MD simulation to investigate both the geometry of D/A interface between two crystals and the D/A blend morphology in self-organized systems (the ordering and molecular orientation, the formation of polythiophene paracrystals and PCBM-rich phases in amorphous regions of polythiophene).

CPP 39.11 Thu 12:30 H34

Electroabsorption spectroscopy on organic pin solar cells — ●ELLEN SIEBERT-HENZE, VADIM G. LYSSENKO, JANINE FISCHER, KARL LEO, and MORITZ RIEDE — Institut für Angewandte Photo-physik, George-Bähr-Str. 1, Dresden, Germany

The built-in voltage has a significant impact on the solar cell performance, but its origins are controversially discussed. In our work we determine the built-in voltage of small molecule organic solar cells based on the pin concept by electroabsorption spectroscopy (EA).

EA detects the change in absorption caused by an electrical field (Stark effect). A change in DC bias on the device results in a variation of the Stark signal. It is probed adding an AC voltage on top of the DC bias enabling the detection using a lock-in amplifier. Thus, the information about the built-in voltage can be evaluated.

As a model system, flat heterojunction solar cells containing C₆₀ as acceptor and MeO-TPD as donor material are investigated. The doping concentration of both the hole and the electron transport layer is modified and it is shown that there is an influence of the consequential change of their work functions on the built-in voltage. Both the short-circuit current as well as the fill factor increase for larger built-in voltages.

CPP 39.12 Thu 12:45 H34

First-principles calculations of the TCO–Organic interface in an OLED — ●ARNO FEY¹, PAUL ERHART², and KARSTEN ALBE¹ — ¹Fachbereich Material- und Geowissenschaften, Technische Universität Darmstadt, Darmstadt, Germany — ²Department of Applied Physics, Chalmers University of Technology, Gothenburg, Sweden

The ongoing development in the field of organic light emitting diode (OLED) technology and the continuously improvement towards higher efficiencies has created a need to understand the interaction between the different layers in an OLED. In this contribution we focus on the interface of the transparent conductive oxide (TCO) and the organic molecule. The interaction between the polar and hydrophilic oxide surface on the one side and the organic and non-polar thin film on the other side determines the growing of the organic film and therefore directly influences the conductivity. The calculations based on the density functional theory (DFT) were carried out using the Vienna ab initio simulation Package (VASP) with Generalized Gradient Approximations (GGA).

CPP 40: Focus: Van der Waals at soft matter interfaces: structure and dynamics

While vdW interactions are successfully taken into account to explain adhesion and repulsion of soft matter at solid interfaces, it is yet not fully understood how dynamic processes are affected. The focus session is aimed to give an overview over recent studies and to address open questions concerning the influence of vdW interactions on structure and dynamics at interfaces including soft matter.

Organizers: Daniela Täuber (Chemnitz) and Karin Jacobs (Saarbrücken)

Time: Thursday 9:30–11:15

Location: H39

Invited Talk CPP 40.1 Thu 9:30 H39
Collective van der Waals Interactions in Molecules, Solids, and Interfaces — ●ALEXANDRE TKATCHENKO — Fritz-Haber-Institut der MPG, Berlin, Germany

Van der Waals (vdW) interactions are ubiquitous in molecules, condensed matter, and hybrid organic/inorganic interfaces. These interactions are inherently quantum mechanical phenomena that arise from concerted fluctuations between many electrons within a given molecular system. Despite this fact, the vast majority of theoretical calculations determine long-range vdW interactions based on a simple effective interatomic pairwise model. We have recently introduced efficient methods that accurately describe the long-range many-body vdW energy for molecules and materials [PRL 108, 236402 (2012); PNAS 109, 14791 (2012); PRL 108, 146103 (2012)]. In this talk, we demonstrate that many-body vdW interactions can successfully explain the recent experimental observations that vdW interactions act at much longer distances than conventionally assumed, and their contribution can significantly exceed the highly coveted “chemical accuracy” for molecules and materials. Our findings suggest that inclusion of the many-body vdW energy is essential for obtaining quantitative and sometimes even qualitatively correct results in materials modeling.

CPP 40.2 Thu 10:00 H39

Enhanced surface tension of liquid–vapour interfaces at mesoscopic scales — ●FELIX HÖFLING and SIEGFRIED DIETRICH — Max Planck Institute for Intelligent Systems, Stuttgart, and Institute for Theoretical Physics IV, Universität Stuttgart, Germany

Due to the simultaneous presence of bulk-like and interfacial fluctuations the understanding of the structure of liquid–vapour interfaces poses a long-lasting and ongoing challenge for experiments, theory, and simulations. In this context, we have generated high-quality molecular dynamics data for a Lennard-Jones fluid mimicking long-ranged van der Waals attraction. Upon lowering the temperature from that of the critical point to that of the triple point, the wavenumber-dependent surface tension develops a maximum at non-zero wavenumber so that its functional form changes from concave to convex at mesoscopic length scales.

Invited Talk CPP 40.3 Thu 10:15 H39
The influence of van der Waals interactions on the adsorption of proteins to solid/liquid interfaces — ●HENDRIK HÄHL — Institute of Physical Chemistry, University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland

Protein adsorption to interfaces is an ubiquitous phenomenon. In particular on solid/liquid boundaries, adsorbed proteins precondition the surface for a later biofilm colonization. Therefore, a better understanding of this first step in biofilm development is highly desirable. The adsorption of proteins to the solid/liquid interface is driven by the interactions between proteins and substrates. Yet, particularly van der Waals (vdW) forces and their dependence on the substrate’s composition are mostly neglected in experiments as well as in simulations.

For the investigation of the influence of vdW forces on protein adsorption, we judiciously chose substrates, with which only the vdW potential could be varied. Therefore, silicon wafers with different sil-

icon oxide thicknesses proved to be an excellent substrate system [1]. Adsorption kinetics as well as the structure of the final adsorbate of several globular proteins were determined on these substrates. Varying the oxide layer thickness caused changes in adsorption rates, course of the adsorption kinetics as well as in the density of the adsorbate irrespective of the surface energy [2]. Thus, it could be shown that the vdW forces between substrate and protein influence the adsorption process and the relaxation of the adsorbate in particular.

[1] P. Loskill et al. *Adv. Coll. Interf. Sci.* **107** (2012) 179182.

[2] H. Hähl et al. *Langmuir* **28** (2012) 7747.

CPP 40.4 Thu 10:45 H39

Influence of van der Waals interactions on morphology and dynamics in ultrathin liquid films at silicon oxide interfaces — ●DANIELA TÄUBER and CHRISTIAN VON BORCZYKOWSKI — nanoMA, TU-Chemnitz, Institut für Physik

Liquids show molecular layering close to interfaces with solids [1]. Its extend is influenced by substrate roughness, humidity and the type of liquid. From studies on wetting behavior, the influence of substrate material on film thickness is known, while also structure formation and dynamics in thin liquid crystal films appeared to depend on the type and thickness of the silicon oxide [2]. Single molecule tracer diffusion studies of evaporating ultrathin tetrakis-2-ethyl-hexoxysilane (TEHOS) films on silicon with 100 nm thermal oxide reveal a slowdown of the tracer mobility 1-2 nm above the substrate [3]. An ellipsometric study of thinning TEHOS films on silicon with 100 nm thermal or 2 nm native oxide yields further information. On the thermal oxide, a lateral flow of the liquid is observed, while the film on the native oxide forms an almost flat surface and shows negligible flow. In addition, we found a significantly smaller initial film thickness in case of the native oxide. We ascribe these differences to van der Waals interactions with the underlying silicon in case of the native oxide, whereas the thermal oxide suffices to shield those interactions [3].

[1] M. L. Forcada, C. M. Mate, *Nature* 363 (1993) 527. [2] B. Schulz, D. Täuber, J. Schuster, T. Baumgärtel, and C. von Borczykowski, *Soft Matter* 7 (2011) 7431. [3] D. Täuber, I. Trenkmann, and C. von Borczykowski, submitted.

CPP 40.5 Thu 11:00 H39

Interface effects on the glass transition temperature in thin supported polymer layers — ●DOMINIK WÖLL^{1,2}, BEATE STEMPELE¹, BENTE FLIER¹, and ANDREAS ZUMBUSCH¹ — ¹Fachbereich Chemie, Universität Konstanz, 78457 Konstanz — ²Zukunftskolleg, Universität Konstanz, 78457 Konstanz

Experimental approaches to study the influence of interfaces on polymer dynamics are challenging. In our contribution, we present wide-field fluorescence microscopy studies to investigate the motion of single dye molecules of different size in thin glass-supported polystyrene films up to temperatures of 150 °C. Heterogeneities in the diffusion coefficients of single molecules were attributed to interface effects influencing the glass transition temperature. Monte Carlo random walk simulations with glass transition temperature profiles taken from literature could rationalize our experimental results, thus confirming that changes in the glass transition temperature at the polymer-air interface can reach only few nm into the polymer film.

CPP 41: Colloids and Complex Liquids I

Time: Thursday 9:30–13:00

Location: H40

Invited Talk

CPP 41.1 Thu 9:30 H40

Out-of-Equilibriumness of Light Activated Colloids — ●JEREMIE PALACCI, STEFANO SACANNA, ASHER PRESKA STEINBERG, ADRIAN VATCHINSKY, KASEY HANSON, DAVID PINE, and PAUL CHAIKIN — NYU, CSMR, USA

Self-propelled micro-particles are intrinsically out-of-equilibrium. This renders their physics far richer than that of passive colloids while relaxing some thermodynamical constraints and give rise to a wealth phenomena e.g. collective behavior, swarming...

I will present various properties of an assembly of synthetic active microparticles. I will notably introduce a new form of self-assembly originating from non-equilibrium driving forces. When activated by light, a set of new self-propelled particles spontaneously assemble into living crystals which behaves as "self-propelled colloidal carpets" steerable with an external magnetic field. We will show that this phenomenon is intrinsically out-of-equilibrium and originates in the competition between self-propulsion, particles collisions and attractive interactions. The applications and the use of this system for colloidal cargo transportation in microfluidic will also be discussed.

CPP 41.2 Thu 10:00 H40

Individually tunable Micromachines driven by laser induced self propelled thermophoresis — ●ANDREAS BREGULLA¹, BIAN QIAN², HAW YANG², and FRANK CICHOS¹ — ¹University of Leipzig, Germany — ²Princeton University

Trapping and guiding individual micro- or nano-objects in solution by optical means is one important task for nanotechnology. Living cells have developed strategies to transport objects with the help of molecular motors. Thus combining active motion with optical control may deliver new pathways for micro and nanomanipulation. Here we present a new concept based on self-thermophoretic action. A particle which is capped by a thin metal layer is heated by a laser beam causing a temperature gradient along the particle surface. This temperature gradient leads to a directed thermophoretic propulsion of the particle. This directed motion, however, is randomized by rotational Brownian motion and just enhanced the diffusive motion on a large timescale. To overcome this randomizing a stochastic feedback mechanism can be developed, which employs the rotational Brownian motion to suppress their action. This method can be extended to the control of multiple individual particles on independent pathways and provides numerous new perspectives for nano-manipulations in liquids.

CPP 41.3 Thu 10:15 H40

Active Brownian motion of asymmetric particles — ●FELIX KÜMMEL¹, IVO BUTTINONI¹, GIOVANNI VOLPE³ und CLEMENS BECHINGER^{2,4} — ^{1,2}Physikalisches Institut, Universität Stuttgart, Germany — ²Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany — ³Bilkent University, Ankara, Turkey

Recently, various systems of active Brownian particles with simple geometries have been studied. Lately, a novel type of spherical active particles being propelled by the local demixing in a binary liquid has been experimentally realized [1]. Here, we investigate the active Brownian motion of asymmetric (L-shaped) particles. We observe an effective torque acting on the particles which results in a circular motion. We investigate this motion both under bulk conditions and close to walls where the torque leads either to the reflection or a sliding along the wall, depending on the direction of the torque. In addition, we investigate the self-propulsion of asymmetric particle under the influence of an external gravitational field. The resulting symmetry breaking causes a gravitactical behavior which strongly depends on the shape and the driving force of the swimmer.

[1] Volpe, G., I. Buttinoni, et al, *Soft Matter* 7, 8810 (2011)

Invited Talk

CPP 41.4 Thu 10:30 H40

Mesoscale Simulations of Active Colloids — ●GERHARD GOMPPER — Institute of Complex Systems, Forschungszentrum Juelich, Germany

Both in soft matter and in biology, there are numerous examples of swimmers and self-propelled particles. With a typical size in the range of a several micro-meters, both low-Reynolds-number hydrodynamics and thermal fluctuations are essential to determine their dynamics. Prominent examples are bacteria like *E. coli* which move forward by a

rotational motion of their spiral-shaped flagella, and synthetic Janus colloids which catalyze a chemical reaction on their surface.

A powerful tool to study the non-equilibrium dynamics of active are mesoscale hydrodynamics simulation techniques, such as multi-particle collision dynamics (MPC), which describe the hydrodynamic behavior of a wide range of complex fluids very well [1].

We focus here on the cooperative behavior of active spherical and rod-like colloids [2], and on the dynamic properties of individual microswimmers near surfaces [3]. Active colloids display a strong surface excess in confined geometries and a pronounced clustering behavior in the bulk. The effects of self-propulsion, hydrodynamic interactions, microswimmer shape, and noise on these phenomena will be discussed.

[1] G. Gompper, T. Ihle, D.M. Kroll, R.G. Winkler, *Adv. Polym. Sci.* 221, 1 (2009).

[2] Y. Yang, V. Marceau, G. Gompper, *Phys. Rev. E* 82, 031904 (2010); I.O. Goetze & G. Gompper, *Phys. Rev. E* 82, 041921 (2010).

[3] J. Elgeti & G. Gompper, *EPL* 85, 38002 (2009).

CPP 41.5 Thu 11:00 H40

Two-dimensional active Brownian motion of asymmetric microswimmers — ●BORGE TEN HAGEN¹, FELIX KÜMMEL², RAPHAEL WITTKOWSKI¹, IVO BUTTINONI², GIOVANNI VOLPE³, CLEMENS BECHINGER^{2,4}, and HARTMUT LÖWEN¹ — ¹Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf — ²Physikalisches Institut, Universität Stuttgart — ³Department of Physics, Bilkent University, Cankaya, Ankara, Turkey — ⁴Max-Planck-Institut für Intelligente Systeme, Stuttgart

We study the Brownian dynamics of asymmetric self-propelled particles in two dimensions. In our theoretical model based on the Langevin equations the propulsion mechanism is taken into account by means of an effective internal force. For asymmetric particles a non-central drive and translation-rotation coupling lead additionally to an effective intrinsic torque. When external forces are neglected, such particles move on a circular trajectory and the noise-averaged trajectory is predicted to be a logarithmic spiral. Under gravity several qualitatively different types of motion are found: Either a straight downward or upward motion (gravitaxis) occurs or the particle describes a periodic circling motion. Our theoretical description, which is very general and holds for arbitrarily shaped microswimmers, is verified in experiments with L-shaped model swimmers.

15 min break

CPP 41.6 Thu 11:30 H40

Swimming trajectory of an active droplet — ●MAX SCHMITT and HOLGER STARK — Institut für Theoretische Physik, TU Berlin

In recent experiments a spherical microswimmer was realized by placing a micron-sized droplet of water and bromine into a surfactant rich oil medium [1]. This active droplet then started to swim in a random direction. However it did not swim in a straight line but rather changed its swimming direction on a timescale much shorter than that of thermal rotational diffusion.

The swimming motion arises due to a chemical reaction of the bromine with the surfactant monolayer at the droplet interface. The reaction product is a surfactant with a higher surface tension. As a consequence, local gradients in surface tension will lead to a fluid flow in the adjacent fluid inside and outside of the droplet. Due to this so-called Marangoni effect, the resting state of the droplet becomes unstable and the droplet starts to move. Simulations of a model in axisymmetric geometry, based on a free energy functional for the droplet interface, confirm the basic swimming motion of the droplet [2].

In a next step we want to explain the increased rotational diffusion relative to the simple thermal diffusion of a sphere. For this we include thermal fluctuations in the surfactant mixture at the interface and omit the axisymmetric constraint. The aim is to connect thermal fluctuations at the interface to the dynamics of the swimming direction of the whole droplet.

[1] Thutupalli S. *et al* 2011 *New J. Phys.* **13** 073021

[2] Schmitt M. and Stark H. 2012 *arXiv* 1210.2560

CPP 41.7 Thu 11:45 H40

Collective dynamics of spherical microswimmers in a quasi-

2D geometry — ●ANDREAS ZÖTTL and HOLGER STARK — TU Berlin
Microorganisms like bacteria, algae or spermatozoa typically move in an aqueous environment where they interact via hydrodynamic flow fields and confining boundaries. Recent experiments studied the collective motion in dense bacterial suspensions where swarming and large-scale turbulence emerged. Moreover, spherical artificial microswimmers, so-called squirmers, have been constructed and studied in a quasi-2D geometry.

First we show that a microswimmer moving in Poiseuille flow in a narrow channel performs van der Pol-like oscillations. Then we present a numerical study of the collective dynamics of squirmers confined in quasi-2D between two parallel walls. Because of their spherical shape the reorientation of squirmers is solely due to noise and hydrodynamic interactions via induced flow fields. This is in contrast to elongated swimmers like bacteria which locally align due to steric interactions.

We study the collective motion of pushers, pullers and potential swimmers at different densities. At small densities the squirmers are oriented parallel to the walls and pairwise collisions determine the reorientation rate. In dense suspensions rotational diffusion is greatly enhanced and pushers, in particular, tend to orient perpendicular to the walls. This effects the dynamics of the emerging clusters. In very dense suspensions we observe active jamming and long-lived ordered structures. The critical area fractions for the formation of crystalline phases is different for pushers, pullers and potential swimmers.

Invited Talk CPP 41.8 Thu 12:00 H40

Orientational Order and Packings of Non-Spherical Particles — ●KLAUS MECKE, RENE WITTMANN, SEBASTIAN KAPFER, and GERD SCHRÖDER-TURK — Institut für Theoretische Physik, FAU, 91058 Erlangen, Germany

Since the seminal work by Y. Rosenfeld in 1989 for fluids of hard spheres a density functional theory is much sought after, which can describe quantitatively hard colloidal particles with arbitrary shapes. A new functional, which is based on fundamental mixed measures known from translative integral geometry, captures nematic and smectic phases correctly and can be used to determine surface tensions and Frank elastic constants.

The bond-orientational order parameter introduced in 1983 by Steinhardt et al. became a standard tool for local structure characterization in colloidal systems, with applications on jamming, crystallization or cluster formation. Unfortunately, the definition of the particle neighborhood significantly affects their interpretation for disordered systems. Mixed measures as well as the related Minkowski tensors can be used to remedy the deficiencies and to characterize local orientational order of non-spherical particles in fluid phases, liquid crystals and also in disordered packings.

CPP 41.9 Thu 12:30 H40

Density functional theory for liquid crystals — ●RENE WITTMANN and KLAUS MECKE — Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany

Fluids of hard spherocylinders exhibit rich phase behavior including isotropic, nematic and smectic phases. The Fundamental Measure Theory for arbitrarily shaped hard particles [1] is applied to this model system within the so-called ζ -approximation.

The spatial homogeneous phases as well as perfectly aligned systems can be treated analytically. Systematically adding higher order terms improves upon the original ζ -correction but remains computationally inefficient for inhomogeneous phases.

We present new results for the phase behavior, the isotropic-nematic interface and the Frank elastic coefficients for the nematic phase. A qualitative comparison with Monte-Carlo simulations confirms the DFT results and for the isotropic-nematic transition we recover the exact Onsager-limit.

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

CPP 41.10 Thu 12:45 H40

Phase behavior of plate-like block copolymer single crystal suspensions — CHUNBO JIANG¹, HAIYING HUANG¹, CUNGUI MA¹, TIANBAI HE¹, and ●FAJUN ZHANG² — ¹State Key Laboratory of Polymer Physics and Chemistry, CIAC, CAS, China — ²Institut für Angewandte Physik, Universität Tübingen

We have studied the influence of particle size and tunable lateral interaction on the isotropic-nematic phase transition of a plate-like colloidal system. The particles are single crystals of a block copolymer PS-b-PLLA prepared using a self-seeding procedure in solutions [1]. These lozenge shape crystals have uniform thickness and narrowly distributed lateral size. The phase behavior is characterized under crossed-polarizers for all systems with size ranging from 500 to 4000 nm. It is surprising to see that the I-N transition occurs at a much lower volume fraction than the theoretical predicted value. However, if adding ethanol into the solution the I-N transition is significantly suppressed. These results demonstrate the existence of a lateral attraction between crystals and it is most likely due to the polar interaction between the crystalline PLLA. Because of the sandwich structure of the crystals, the confinement by the amorphous PS layers renders the attraction highly orientation dependence. In this way, larger plate-sheets are formed via lateral attraction and give a much lower critical volume fraction. To further demonstrate this highly orientational attraction, we have further prepared a composite single crystal with a PLLA homopolymer. Indeed, the resulting liquid crystalline phases show much less horizontal ordering. [1] Jiang C. et al. Langmuir 2011, 27, 4351

CPP 42: New Instruments and Methods

Time: Thursday 11:30–13:00

Location: H39

CPP 42.1 Thu 11:30 H39

Design of neutron spin-echo spectrometers for ESS — ●STEFANO PASINI¹, MICHAEL MONKENBUSCH¹, and MELISSA SHARP² — ¹Jülich Center for Neutron Science, FZJ, Germany — ²ESS AB, Lund, Sweden

Neutron spin echo (NSE) is the technique with the highest energy resolution for probing the dynamics of materials. Within the German European Spallation Source design update project, the Research Centre Jülich is optimizing a high-resolution (HRNSE) and a wide-angle neutron spin-echo (WANSE) spectrometer. The specifications of the polarization system will be analogous for both instruments: A straight, 8cmx8cm neutron guide with a comparatively short (~2.6m) polarizing bender or eventually a single polarizing mirror inducing a kink in the guide. A potential beam extension and focusing in horizontal direction for the WANSE is still under investigation. For the design of the magnetic layout of the HRNSE, we combined the active stray field compensation techniques used at the SNS-NSE, enabled by superconducting coils, and a coil-geometry optimization versus minimization of field-integral inhomogeneity, depolarization and stray-field. We found a solution with 3 times reduced intrinsic inhomogeneity of field integrals and low stray fields allowing for a working configuration up to

2Tm field integral. The limitations of the correction elements will be partly resolved by the increased field homogeneity. The strategy of low intrinsic inhomogeneity has been pursued also for the WANSE. This should allow us to reach a resolution comparable with that of the current high resolution J-NSE@FRM-II.

CPP 42.2 Thu 11:45 H39

Combining advanced sputter deposition and GISAXS - new avenues for in-situ experiments — RALPH DOEHRMANN¹, GUNTARD BENECKE^{1,2}, SEBASTIAN BOMMEL¹, STEPHAN BOTTA¹, BERIT HEIDMANN¹, GERD HERZOG¹, ROMAN MANNWEILER¹, JOHANNES RISCH¹, MATTHIAS SCHWARTZKOPF¹, GONZALO SANTORO¹, SHUN YU¹, and ●STEPHAN VOLKHER ROTH¹ — ¹Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, D-22607 Hamburg, Germany — ²MPI Colloids and Interfaces Golm, Abt. Biomat., Wissenschaftspark Potsdam-Golm, D-14424 Potsdam, Germany

Nanocomposite structures play an important role in organic photovoltaics. To elucidate their structure-function relationship and to tailor them on the nanoscale, in-situ investigations following their formation are mandatory. These investigations have to cover the nano/molecular level to the mesoscale domain. This necessitates the use of scattering techniques like small- and wide angle x-ray scattering. Sputter

deposition often is the final step in producing an electric contact in organic photovoltaic devices. We present a novel in-situ sputter deposition chamber for grazing incidence small- and wide-angle x-ray scattering investigations using microfocused x-ray beams [1,2]. We present first results of in-situ metal sputter deposition on inorganic and polymeric surfaces, using its unique high-temperature annealing and high-throughput capacities. This allows for the first time combinatorial in-situ microbeam GISAXS investigations to scan the parameter range during sputter deposition. [1] Roth et al., J. Phys: Cond. Matter 23, 254208 (2011) [2] Buffet et al., J. Synchr. Radiation 19, 647 (2012)

CPP 42.3 Thu 12:00 H39

Nanocharacterization of Organic Semiconductors using NanoXAS, a Combined Scanning Transmission X-ray Microscopy/Scanning Probe Microscopy instrument — PETER WARNICKE¹, NICOLAS PILET¹, BENJAMIN WATTS¹, RAINER FINK², CHRISTOPH QUITMANN¹, and JÖRG RAABE¹ — ¹Paul Scherrer Institut, 5232 Villigen, Switzerland — ²Univ. Erlangen-Nürnberg, 91058 Erlangen, Germany

Properties of organic semiconducting materials are strongly linked to the interplay between chemical composition and microstructure. As techniques providing simultaneous information on these characteristics are lacking there is a great need for more complete characterization tools. Here we present a novel instrument (NanoXAS) which combines two powerful techniques, scanning probe microscopy (SPM) and x-ray absorption spectroscopy (XAS), in order to fully characterize organic semiconducting materials and devices. SPM can measure physical properties such as sample topography, elasticity, adhesion, or friction on lateral scales down to nanometers. XAS gives direct access to the local chemical composition, electronic structure, molecular orientation, order, and absolute density. The instrument consists of a SPM and a scanning transmission x-ray microscope (STXM) in a coaxial arrangement. A semi-transparent sample is scanned through the x-ray beam and the transmitted x-rays are detected by a photodiode or by a SPM tip thus enabling high-resolution imaging with element sensitivity. To demonstrate the function of the instrument we present measurements on polymers and polymer blends.

CPP 42.4 Thu 12:15 H39

Confocal and polarized μ -RAMAN Imaging-Spectroscopy as a tool for the estimation of crystallinity and orientation of iPP films and Pirouette rings — KRISZTINA VINCZE-MINYA¹, SABINE HILD¹, SIBYLLE JILG², and REINHARD FORSTNER² — ¹Institute of Polymer Science, Johannes Kepler University, Linz, Austria — ²TCKT - Transfer Center for Polymer Technology GmbH, Wels, Austria

The morphology of iPP polypropylenes strongly depends on conditions of sample preparation. While stretching and temperature induced changes in polymer microstructure are widely explored the influence of shear stress is only sparsely investigated. Pirouette-dilatometer enable to prepare samples at defined temperature, pressure and cooling conditions may show local variations in crystallinity and orientation. Polarized confocal Raman microscopy (pCRM) will be used to investigate local variation crystallinity and orientation of iPP samples sheared by Pirouette-dilatometer. Therefore, pCRM imaging was applied on iPP cast and MDO films, which have an orientation measured via WAXS revealing the suitability of the method for the investigation of

crystallinity and orientation with high spatial resolution. The Hermans orientation function was as well estimated and found to be also in good correlation with the WAXS data. Cast films: high depolarization ratio, low orientation, higher crystallinity degree. MDO films: low depolarization ratio, high orientation, lower crystallinity degree. The slow cooled Pirouette-samples have a lower crystallinity than the fast cooled samples, and the differences between the stretch and unstretched samples are also presented.

CPP 42.5 Thu 12:30 H39

Larmor precession in ultralow magnetic fields detected by Field Cycling NMR — BENJAMIN KRESSE — Institut für Festkörperphysik, TU Darmstadt, Hochschulstr. 6, 64289 Darmstadt

Field Cycling (FC) relaxometry is a powerful tool to measure the microscopic dynamics at a wide range of Larmor frequencies. Typically, the highest accessible magnetic field of about 1 Tesla is limited by the power of the magnet, while the low frequency limit is the noise of the current source. The present work deals with experiments in the low frequency range.

For reaching low magnetic fields in an FC experiment it is important to (i) compensate the earth field, (ii) avoid a zero field overshoot during the fast field switch from high to low field, (iii) stabilize the low field and (iv) measure the low field at the sample position.

Our way to solve these problems is to implement a set of five independently controlled coils into our home built FC magnet. This setup allows us to perform non-adiabatic field switch down to a low evolution field which is controlled by an active fluctuation compensation. In a series of test experiments the lowest stable magnetic field we reached and measured directly by Larmor precession of protons in a water sample was about 0.3 microTesla corresponding to $\nu_0(^1H) = 12$ Hz [B. Kresse, A. Privalov, F. Fujara / Solid State Nuclear Magnetic Resonance 40 (2011) 134-137]. With this setup it is also possible to measure T_1 and the evolution field combined in one and the same measurement.

CPP 42.6 Thu 12:45 H39

Pseudo-critical behavior of the static and the dynamic expansion coefficient at the volume phase transition of PNIPAM solutions as seen by Temperature Modulated Optical Refractometry — RALITSA ALEKSANDROVA¹, MARTINE PHILIPP^{1,2}, ULRICH MÜLLER¹, ROLAND SANCTUARY¹, PETER-MÜLLER BUSCHBAUM², and JAN K. KRÜGER¹ — ¹Université du Luxembourg, LPM, Luxembourg, Luxembourg — ²TU München, Physik-Department, LS Funktionelle Materialien, Garching, Germany

The volume phase transitions of aqueous PNIPAM solutions are investigated by the novel technique of Temperature Modulated Optical Refractometry (TMOR) as a function of temperature and time. In addition to the refractive index, TMOR yields information about the static and dynamic thermo-optical coefficient and eventually the static and dynamic volume coefficient of thermal expansion [1]. The observed pseudo-critical behavior of these physical quantities evidences a rather direct coupling to the order parameter associated with the collapse of the polymer coils. A preliminary interpretation with regard to the involved structural changes on mesoscopic and macroscopic scales is given based on these findings.

[1] M. Philipp, U. Müller, R. Aleksandrova et al., Soft Matter 8, 11387 (2012)

CPP 43: Organic Electronics and Photovoltaics V (joint session CPP/HL/O/DS)

Time: Thursday 15:00–18:45

Location: H34

Invited Talk

CPP 43.1 Thu 15:00 H34

Quantum coherence controls the charge separation in a prototypical artificial light harvesting system — C. LIENAU¹, S. M. FALKE¹, C. A. ROZZI², N. SPALLANZANI², A. RUBIO², E. MOLINARI², D. BRIDA³, M. MAIURI³, G. CERULLO³, H. SCHRAMM⁴, and J. CHRISTOFFERS⁴ — ¹Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany — ²Istituto Nanoscienze - CNR, Centro S3, Modena, Italy — ³IFN-CNR, Dipartimento di Fisica, Politecnico di Milano, Italy — ⁴Institut für Reine und Angewandte Chemie, Carl von Ossietzky Universität Oldenburg, Germany

The efficient conversion of light into electricity or chemical fuels is a fundamental challenge. In artificial photosynthetic and photovoltaic

devices this conversion is generally thought to happen on ultrafast time scales in the fs to ps range and to involve an incoherent electron transfer process. In some natural biological systems, however, there is now growing evidence that the coherent motion of electronic wavepackets is an essential primary step, raising questions about the role of quantum coherence in artificial devices. Here we investigate the primary charge transfer process in a supramolecular triad, a prototypical artificial reaction center. Combining high time-resolution femtosecond spectroscopy and time-dependent density functional theory, we provide compelling evidence that the driving mechanism of the photoinduced current generation cycle is a correlated wavelike motion of electrons and nuclei on a timescale of few tens of femtoseconds. We highlight the fundamental role of the interface between chromophore and charge acceptor in

triggering the coherent wavelike electron-hole splitting.

CPP 43.2 Thu 15:30 H34

Simulations of Electron Transfer in a Fullerene Hexa-Pyropheophorbide-a Complex — •THOMAS PLEHN, JÖRG MEGOW, and VOLKHARD MAY — Humboldt-Universität zu Berlin, Germany

Electron transfer (ET) is studied between electronically excited chromophores and a C60 fullerene forming a highly flexible complex, which is dissolved in a solvent. Such investigations are of particular interest with regard to future artificial photosynthetic reaction centers and respective applications in future components of photovoltaic devices. The whole discussion is based on extended MD-simulations. To obtain reliable ET results three differently advanced theories are used. The first treatment uses the classical Marcus theory. Respective Marcus parameters are obtained from literature [1]. A generalized ansatz can be derived by the Landau-Zener theory [2]. Secondly, a semi-classical surface-hopping method [3] is chosen. For this approach the conformation-dependent free-energy surfaces and Marcus parameters are calculated directly from the MD-trajectory. The third approach uses the dispersed-polaron/spin-boson model [3]. This method enables the approximation of a quantum-mechanical harmonic oscillator bath and thus the treatment of nuclear tunneling. A comparative discussion of the outcome of these three methods also in relation to experiment [1] is given finally.

[1] Regehly M. et al., J. Phys. Chem. B 2007, 111, 998

[2] Hlczar M. et al., J. Photochem. Photobiol. A 2003, 158, 83

[3] Warshel A. et al., Q. Rev. Biophys. 2001, 34, 4, 563

CPP 43.3 Thu 15:45 H34

Highly conductive PEDOT:PSS for flexible structured ITO-free solar cells — •CLAUDIA M. PALUMBINY¹, CHRISTOPH HELLER¹, ROBERT MEIER¹, GONZALO SANTORO², STEPHAN V. ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str.1, 85747 Garching, Germany — ²HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany

PEDOT:PSS is widely used as selective intermediate electrode in flexible electronics. The mechanical stability of the electrodes yet play a crucial role and is limited by the instability of the ITO/FTO electrode and the low conductivity of PEDOT:PSS. We investigate a recently developed post treatment method enhancing the conductivity of PEDOT:PSS reaching the order of ITO. For a deeper understanding the nanomorphology is investigated with surface imaging techniques (AFM, SEM) and the inner morphology and crystallinity is addressed with GISAXS and GIWAXS. The morphological changes are consequently related to the electronically changes. Furthermore, we introduce a novel structuring routine for PEDOT:PSS, plasticizer assisted soft embossing [1]. Being able to control the interface between the transparent electrode and the active material, the device efficiency of OPVs under oblique light can be increased. Combining highly conductive PEDOT:PSS with controlled structuring, these results reveal new paths for flexible structured ITO-free solar cells of enhanced efficiency.

[1] R. Meier, C. Birkenstock, C.M. Palumbiny and P. Müller-Buschbaum, Phys. Chem. Chem. Phys., 14, 15088-15098 (2012)

CPP 43.4 Thu 16:00 H34

Electropolymerized polythiophenes as contact layers in organic solar cells — •SIDHANT BOM and VEIT WAGNER — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Electropolymerized thiophene offers additional advantages to solution processable thiophenes because the doping concentration can be controlled with electrical parameters. The in-situ electrochemical doping provides a handle for the optimization of organic solar cells, either as a bulk polymer in the active layer or as an electron blocking layer. Here in this study, thiophenes are grown electrochemically with a standard three electrode system on Indium Tin Oxide (ITO) contacts. Characterization by UV-Vis measurements reflects the tunable final oxidation state of the thiophene layer. Thin layers are used in diode configuration using metal contacts like Au, Ag, Al and Cu. Static IV measurement allows the characterization of the contact according to Schottky model. Impedance measurements are used to determine the doping level of the layer. The doping level is found to be systematically depending on the applied negative bias during growth at the working ITO electrode with respect to the counter electrode. Applying a negative bias for a short interval at the end of the growth results in highly doped layers which are suitable for contact layers in solar cells.

CPP 43.5 Thu 16:15 H34

Efficient solution processed p-type doping for OLEDs — •CHRISTIAN TÖPEL, THORSTEN UMBACH, ANDRÉ JOPPICH, JEANETTE BÖCKMANN, ANNE KÖHNEN, and KLAUS MEERHOLZ — University of Cologne, Chemistry Department

Organic light emitting diodes (OLEDs) have drawn much attention in science and industry. Application such as new generation lighting and display devices contribute strongly. However, drawbacks are inefficient charge carrier injection into and low conductivity of the organic materials. A promising solution for this problem is molecular doping which is commonly used in vacuum processed OLEDs, yielding in highly efficient luminescent devices (pin concept). In this case, the molecular doping leads to partial redoxchemical doping. As vacuum deposition is very cost intensive and does not allow high volume processing, researchers focus more and more on solution processing. Here, we present efficient molecular p-type doping using various crosslinkable small-molecule hole transporting materials combined with a range of molecular dopants. Unipolar devices feature an increase in current density by several orders of magnitude compared to the undoped devices at the same voltage. We will also introduce these layers into all-solution-processed multiple-layer OLEDs. These devices are compared with their vacuum-processed counterparts to show the influence of the deposition method and doping ratio on OLED lifetime and device performance.

CPP 43.6 Thu 16:30 H34

Degradation induced decrease of the radiative quantum efficiency in organic light-emitting diodes — •TOBIAS D. SCHMIDT¹, DANIEL S. SETZ², MICHAEL FLÄMMICH³, BERT J. SCHOLZ¹, ARNDT JAEGER², CAROLA DIEZ², DIRK MICHAELIS³, NORBERT DANZ³, and WOLFGANG BRÜTTING¹ — ¹Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — ²OSRAM Opto Semiconductors GmbH, Leibnizstrasse 4, 93055 Regensburg, Germany — ³Fraunhofer Institute for Applied Optics and Precision Engineering, 07745 Jena, Germany

The efficiency decrease during electrical operation of organic light-emitting diodes is a crucial issue for both applied and fundamental research. In order to investigate degradation processes, we have performed an efficiency analysis for phosphorescent state-of-the-art devices in the pristine state and after an accelerated aging process at high current density resulting in a luminance drop to less than 60 % of the initial value. This loss in efficiency can be explained by a decrease of the radiative quantum efficiency of the light-emitting guest/host system from 70 % to 40 %, while other factors determining the efficiency are not affected.

15 min. break

CPP 43.7 Thu 17:00 H34

Enhanced light outcoupling from corrugated top-emitting OLEDs — •C. FUCHS¹, T. SCHWAB¹, A. ZAKHIDOV^{1,2}, K. LEO¹, M. C. GATHER¹, and R. SCHOLZ¹ — ¹Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr Str. 1, 01069 Dresden — ²Fraunhofer COMEDD, Maria-Reiche-Str. 2, 01109 Dresden

We analyse the emission spectra of phosphorescent top-emitting OLEDs grown on corrugated substrates. The corrugation is produced using photolithography. Thereby photoresist, spin-coated on a glass substrate is illuminated by an incoherent UV source across a contact mask with periodic structures in the sub- μm range. The optical microcavity of the OLED grown on top is defined by a thick metallic bottom contact, organic layers following the p-i-n concept, a thin metallic top contact, and an organic capping layer maximizing the outcoupling efficiency. Depending on the periodicity of the substrate, Bragg scattered wave guide modes may interfere constructively or destructively with the cavity mode inside the air light cone, hence enhancing or decreasing light emission with respect to a planar microcavity. Thus, the emission pattern deviates strongly from a Lambertian shape, but the angle-integrated external quantum efficiency can be enhanced by up to a factor of about 1.2 with respect to a fully optimized planar reference. Besides a quantitative assignment of sharp features in the emission spectra, an analysis of Bragg scattering for different periodicities can be used for designing a particular angular emission pattern, e.g. very strong forward characteristics.

CPP 43.8 Thu 17:15 H34

Characterization of Gravure Printed Polymer Light-Emitting Electrochemical Cells — ●GERARDO HERNANDEZ-SOSA, RALPH ECKSTEIN, SERPIL TEKOGU, FLORIAN MATHIES, ULI LEMMER, and NORMAN MECHAU — Lichttechnisches Institut, Karlsruher Institut für Technologie, Karlsruhe, Deutschland

In this work we present the fabrication, characterization and ink formulation of gravure printed polymer light-emitting electrochemical cells (LECs). These light emitting devices are fabricated by sandwiching a blend of a semiconducting polymer with a solid polymer electrolyte (SPE) between two electrodes, regardless of their work function. When applying a voltage to the device, the ionic species in the active film will help to form p or n doped layers at the corresponding electrode. Following the injection of carriers, the light emission will come from the semiconductor through the formation and successive recombination of excitons in the intrinsic layer between the p and n doped regions. We correlate the LEC ink formulation to the film quality and device performance. The properties of the formulation are characterized by viscosity and contact angle measurements while the properties of the film are studied by impedance spectroscopy and atomic force microscopy.

CPP 43.9 Thu 17:30 H34

Strongly Fluorescent Copper Complexes for Application in OLEDs Using the Singlet-Harvesting Effect — ●RAFAL CZERWIENIEC and HARTMUT YERSIN — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, D-93040, Germany.

A series of strongly luminescent Cu(I) complexes is presented. The emissions cover a broad spectral range from the blue to the orange. The ambient temperature quantum yields are as high as 90 % and the decay times lie in the order of several microseconds. From a detailed analysis of the photophysical behavior, the ambient temperature emission is assigned to a thermally activated delayed fluorescence (TADF). This is in contrast to the situation at low temperatures, e.g. below 100 K, at which the emission stems from the lowest triplet state decaying as long-lived phosphorescence (order of several hundred microseconds). The observed photophysical properties are related to small energy separations between the S_1 (singlet) and T_1 (triplet) excited states. The results demonstrate the high potential for application of these materials as OLED emitters by exploiting the recently reported singlet harvesting mechanism.

Literature:

1. R. Czerwiec, J. Yu, H. Yersin, *Inorg. Chem.*, 2011, 50, 8293-8301.
2. H. Yersin, A. F. Rausch, R. Czerwiec, T. Hofbeck, T. Fischer, *Coord. Chem. Rev.*, 2011, 255, 2622-2652.

CPP 43.10 Thu 17:45 H34

Insight into the photophysics of photocatalytically active polymeric carbon nitride: an optical quasi-monomer — ●CHRISTOPH MERSCHJANN¹, TOBIAS TYBORSKI^{1,2}, STEVEN ORTHMANN^{1,3}, FLORENT YANG¹, KLAUS SCHWARZBURG¹, MICHAEL LUBLOW^{1,4}, and THOMAS SCHEDEL-NIEDRIG¹ — ¹Helmholtz-Zentrum-Berlin für Materialien und Energie — ²Max-Born-Institut für nichtlineare Optik und Kurzzeitspektroskopie, Berlin — ³Technische Universität Berlin — ⁴Leibnitz-Institut für Katalyse, Rostock

A comprehensive investigation of the luminescent properties of photocatalytically active carbon nitride polymers, based on tri-s-triazine units, has been conducted for the first time. Steady-state temperature- and excitation-power-dependent as well as time-resolved measurements with near-UV excitation ($\lambda = 325 \text{ nm}$ & 405 nm) yield strong photoluminescence, covering the visible spectrum. The spectral, thermal and temporal features of the photoluminescence can be satisfactorily described by the excitation and radiative recombination of molecular excitons, localized at single tri-s-triazine units. The discussed model is in accordance with the recently reported absorption features of carbon nitride polymers. Thus, from the point of view of optical spectroscopy, the material effectively behaves as a monomer rather than a classical semiconductor.

CPP 43.11 Thu 18:00 H34

Polymer semiconductors for electro chemical measurements in biosensing applications — ●MARTIN SCHMID — Helmholtz Zentrum München, Munich, Germany

There is an increasing need in medical diagnosis for reliable fast and simple biosensing devices. Sensors based on organic semiconducting polymers, which are suitable for large-area, low-cost, flexible, and eventually single-use throwaway electronics, provide a unique opportunity in that sense. We report on organic field-effect transistors (OFETs) with regioregular poly(3-hexylthiophene) (P3HT) operable at low-voltages in liquid solutions, suitable for in vitro biosensing applications. Measurements in electrolytes have shown that the performance of the transistors did not deteriorate and they can be directly used as ion-sensitive transducers. Here we show the detection of pH alterations in a wide linear range. With the intention to use the sensors as biosensing devices in biomedical applications, the experiments were performed under physiological conditions and temperature.

CPP 43.12 Thu 18:15 H34

Magnetoresistive Field-Effect Transistors based on Spiro-TAD/Spiro-PFPy Donor/Acceptor-Blends — ●THOMAS REICHERT, CAROLIN ISENBERG, TOBAT 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, 34132, Kassel, Germany.

One promising opportunity for the realization of next generation magneto-optoelectronic devices is the use of the electron spin as an additional control parameter. In organic semiconductors the spin states of quasiparticles can be adjusted with low magnetic fields, which leads to large (up to 20% at 10mT) magnetoresistive effects at room temperature. We show that the sign of magnetoresistance (MR) in organic field-effect transistors (OFETs) can be tuned from positive to negative by simply applying illumination. In darkness an external magnetic-field increases the resistance (positive MR) while a magnetic-field induced resistance decrease (negative MR) can be achieved under illumination. The key aspect of this promising effect is the application of co-evaporated Spiro-TAD/Spiro-PFPy blends as the charge transport layers in OFETs. Due to the hole (electron) stabilizing properties of Spiro-TAD (Spiro-PFPy) a mixed donor/acceptor blend is formed, which leads to the observed photoinduced MR sign change. This effect can pave the way to future multifunctional spintronic devices.

CPP 43.13 Thu 18:30 H34

In-wire device: combination of organic semiconductors with electrodes in an individual nanowire — ●CHENGLIANG WANG, HUAPING ZHAO, LIAOYONG WEN, YAN MI, and YONG LEI — Fachgebiet 3D-Nanostrukturierung, Institut für Physik & IMN MacroNano* (ZIK), Technische Universität Ilmenau, Prof. Schmidt Str. 26, 98693 Ilmenau, Germany

One-dimensional wires constituted with kinds of segments attracted much attention due to their potential application in nanogaps obtained from on-wire lithography, plasmonic disk arrays, optimized Raman *hot spots* and heterojunction structures¹. Here, we will talk about the in-wire device, which combined the organic semiconductor and the electrodes in an individual nanowire, based on anodic alumina oxide (AAO) template²⁻³. This kind of nanodevice could be applied in organic diodes, transistors or memories, which attracted extensive attention due to the flexibility, the ease to be functionalized, the colorful and the low cost⁴.

Reference:

- [1] S. J. Hurst, E. K. Payne, L. Qin, C. A. Mirkin, *Angew. Chem. Int. Ed.* 2006, 45, 2672.
- [2] Y. Lei, S. Yang, M. Wu, G. Wilde, *Chem. Soc. Rev.* 2011, 40, 1247.
- [3] Y. Lei, W. Cai, G. Wilde, *Progress in Materials Science* 2007, 52, 465.
- [4] C. Wang, H. Dong, W. Hu, Y. Liu, D. Zhu, *Chem. Rev.* 2012, 112, 2208.

CPP 44: Wetting, Micro- and Nanofluidics

Time: Thursday 15:00–18:45

Location: H39

Invited Talk

CPP 44.1 Thu 15:00 H39

Dynamic reorganization of droplets: from Foams to Phonons — ●RALF SEEMANN^{1,2}, JEAN-BAPTISTE FLEURY¹, ULF D. SCHILLER³, SHASHI THUTUPALLI², OHLE CLAUSSEN², STEPHAN HERMINGHAUS², GERHARD GOMPPER³, and MARTIN BRINKMANN^{1,2} — ¹Experimental Physics, Saarland University, Germany — ²MPI for Dynamics and Self-Organization, Göttingen, Germany — ³Theoretical and Soft Matter Biophysics, FZ Jülich, Germany

The stability and the mechanical response of monodisperse droplet packing in quasi 2d micro-channels are discussed for different packing density under static and dynamic conditions: Very dense droplet arrangements are analogous to foam and can be described by geometrical means provided the friction with the side walls is low. At reduced droplet fraction where the droplets are still in mechanical contact, the resulting droplet arrangements are stabilized by virtue of the Laplace pressure. Depending on the exact choice of parameter a droplet packing can have a negative compressibility separating into stable domains of higher and lower packing fraction. When flowing along a microfluidic channel these unstable droplet arrangements develop complex non-equilibrium re-arrangements similar to avalanches. Reducing the droplet fraction even further so that the droplets do not touch each other, the flowing droplets experience each other by dipole-like hydrodynamic interactions and can be excited to show collective oscillations which can be described by a phonon-type behavior.

CPP 44.2 Thu 15:30 H39

Optimal Particle Separation in Microfluidic Systems Using Inertial Lift Forces — ●CHRISTOPHER PROHM and HOLGER STARK — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin, Germany

At intermediate Reynolds numbers, particles in a microfluidic channel assemble at fixed distances from the channel axis and bounding walls [1]. This Segré-Silberberg effect can be described in terms of an effective lift force acting on the particles.

Devices utilizing inertial lift forces for the separation of bacteria and red blood cells have recently been demonstrated [2]. The separation is most efficient for large size differences since the inertial lift force scales with the third power of the particle radius.

Here, we show that one can use external forces generated, for example, by optical tweezers to separate particles similar in size. We determine the inertial lift force by mesoscopic simulations [3] and use it to set up a Smoluchowski equation which describes the particle motion in lateral direction. We then employ the formalism of optimal control [4] to determine profiles of the external force, which help to steer particles and thereby maximize particle separation.

[1] G. Segré and A. Silberberg, *Nature*, **189**, 209 (1961).

[2] A. J. Mach and D. Di Carlo, *Biotechnol. Bioeng.*, **107**, 302 (2010).

[3] C. Prohm, M. Gierlak, and H. Stark *EPJE*, **35**, 80 (2012).

[4] F. Tröltzsch, *Optimal Control of Partial Differential Equations*, American Mathematical Society, first edition (2010).

CPP 44.3 Thu 15:45 H39

Microfluidic Rocking ratchet for the separation of magnetically labeled cells — ●LARS HELMICH¹, MATTHIAS SCHUERMANN², ALEXANDER AUGE¹, FRANK WITTBRAUCHT¹, CHRISTIAN KALTSCHMIDT², and ANDREAS HUETTEN¹ — ¹Thin films and Physics of Nanostructures, Department of Physics, Bielefeld University — ²Department of Cell Biology, Bielefeld University

The aim of so called lab-on-a-chip devices is to integrate all laboratory tasks on one microfluidic chip. Employing magnetic materials particularly magnetic beads in these systems has gained great interest during the last decades [1,2].

One way of controlling and directing the motion of magnetically functionalized particles is the use of Rocking ratchet structures [3].

We present a separation device consisting of a micro structured spatially periodic array of conduction lines beneath a microfluidic channel and an additional external magnetic gradient field. Human embryonic kidney cells were labeled with magnetic beads. Depending on the choice of field strengths and switching times it is possible to separate cells by diffusivity and magnetic moment. Parameter optimization studies were carried out by means of finite element method based numerical simulations.

[1] A. Auge et al., *Appl. Phys. Lett* **94**, 183507 (2009)

[2] N. Pamme, *Lab On A Chip*, **6**(1) 24-38 (2006)

[3] P. Reimann, *Physics Reports*, **361** 57-265 (2002)

CPP 44.4 Thu 16:00 H39

Fluctuating Boundary Conditions in Hydrodynamics — ●MARTIN REICHELDORFER and KLAUS MECKE — Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen

Fluctuating internal stresses are ubiquitous in the hydrodynamics of small systems. The correlations of these ‘noise’ terms are closely related to the viscosities, which is an example of a fluctuation dissipation relation. Here, we extend this fundamental principle to fluid interfaces with slip boundary conditions. We demonstrate that fluid-fluid and fluid-substrate interactions can be treated consistently in a unified way by introducing a fluctuating boundary force. In the spirit of Bocquet and Barrat [1] the correlations of the latter give rise to the friction coefficient between fluid and substrate. Moreover, we show that cross-correlations with the fluctuating stresses inside the liquid can lead to even strongly enhanced slip, described by an effective slip length. As an application we study the dewetting dynamics of thin liquid films [2].

[1] L. Bocquet and J.-L. Barrat. *Physical Review E*, **49**(4):3079, 1994.

[2] R. Fetzer et al. *Physical Review Letters*, **99**:114503, 2007.

CPP 44.5 Thu 16:15 H39

Influence of Slip on the Rayleigh-Plateau Rim Instability in Dewetting Polymer Films — ●SABRINA HAEFNER¹, OLIVER BÄUMCHEN^{1,2}, LUDOVIC MARQUANT¹, MATTHIAS LESSEL¹, RALF BLOSSEY³, ANDREAS MÜNCH⁴, BARBARA WAGNER⁵, and KARIN JACOBS¹ — ¹Saarland University, Experimental Physics, D-66041 Saarbrücken, Germany — ²McMasters University, Dept. of Physics & Astronomy, Hamilton, ON, Canada — ³Interdisciplinary Research Institute (IRI), CNRS USR 3078, Villeneuve — ⁴Mathematical Institute, University of Oxford, Oxford OX1 3LB, UK — ⁵Technical University of Berlin, Institute for Mathematics, 10623 Berlin, Germany

A dewetting polymer film develops a characteristic fluid rim at its receding edge due to mass conservation. In the course of the dewetting process the rim becomes unstable via an instability of Rayleigh-Plateau type. An important difference exists between this classic instability of a liquid column and the rim instability in the thin film as the growth of the rim is continuously fueled by the receding film. We explain how the development and macroscopic morphology of the rim instability are controlled by the slip of the film on the substrate. A single thin-film model, valid for all slip lengths, captures quantitatively the characteristics of the evolution of the rim observed in our experiments.

CPP 44.6 Thu 16:30 H39

Self-Similarity and Energy Dissipation in Stepped Polymer Films — ●JOSHUA D. MCGRAW¹, THOMAS SALEZ², OLIVER BÄUMCHEN¹, ELIE RAPHAËL², and KARI DALNOKI-VERESS¹ — ¹Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada — ²Laboratoire de Physico-Chimie Théorique, UMR CNRS Gulliver 7083, ESPCI, Paris, France

We have recently learned how to prepare polymer films whose only feature is a step in the height profile [1]. In the melt, Laplace pressure drives a flow that levels the topography, with the excess energy of the height step being dissipated by viscosity. It has been observed that the profiles are self-similar in time for a variety of molecular weights and geometries. Given the surface tension, this simple observation allows a precise measurement of the viscosity by comparison with numerical solutions [2] of the thin film equation. It is also possible to derive a master expression for the time dependence of the excess surface energy as a function of the material properties and film geometry. Thus, all geometries and molecular weights fall on a single temporal curve. The material parameter allowing this collapse is the capillary velocity: the ratio of the surface tension to the viscosity.

[1] McGraw et al., *PRL* (2012).

[2] Salez et al., *EPJE* (2012).

15 min. break

Invited Talk

CPP 44.7 Thu 17:00 H39

Wetting behaviour in inkjet printed droplets — ●PATRICK SMITH and JONATHAN STRINGER — University of Sheffield, Krotov Research Institute, Broad Lane, Sheffield, S3 7HQ, England

Understanding how droplets behave is essential to using inkjet printing if inkjet is to be successful as a manufacturing process. This talk discusses the lifetime of droplets from when they are ejected from a nozzle, their impact with a substrate and their drying behaviour.

In this contribution I will discuss how, by varying the height of a printhead nozzle above a substrate, the final dried droplet diameter of a polymer ink can be decreased. I will also show that at higher concentrations of polymer, the solute forms a skin on the surface of the inkjet printed droplet, which inhibits the in-flight evaporation of the solvent. I will also discuss a study into the spreading of inkjet printed droplets of a polystyrene/toluene solution with varied molar masses on solid dry surfaces. The experimental results were compared to theoretical models and found to have a good fit. The spreading factor was found to decrease as molar mass increased, which is explained in terms of increased viscosity. Finally, I will discuss how the size of a suspended particle can influence the size of the final dried morphology of a printed feature.

CPP 44.8 Thu 17:30 H39

Marangoni Modified Drop Fusion and Drop Motion — ●STEFAN KARPITSCHKA and HANS RIEGLER — MPI für Kolloid- und Grenzflächenforschung, Potsdam, Germany

Sessile droplets on solid surfaces will fuse due to capillary forces. The droplet fusion can be delayed if the droplets consist of different (but still completely miscible) liquids. Quite unexpected, even after initial contact at the three phase line, the main droplet bodies remain separated. The droplets are connected only through a neck via a thin liquid film and move together over the substrate surface [1]. This non-coalescing state can last up to minutes. Its origin are the different surface energies of the liquids: The difference induces a Marangoni flow between the droplets which keeps them separate [2]. Based on new experiments, we present – for the first time – an analytical treatment in the framework of a thin film description. The key ingredient is a balance of advective and diffusive transport mechanisms in the vicinity of the neck, which induces a Marangoni flow. By piece-wise asymptotic matching of meso- and microscopic solutions we determine the global free surface topology and the capillary number [3]. We find traveling wave solutions in quantitative agreement with the experimental observations. The findings are generally relevant for (shallow, steady-state) free surface flows that involve (are caused by) surface tension gradients (e.g. due to local compositional variations).

[1] H. Riegler, P. Lazar, *Langmuir* 24, 6395 (2008).

[2] S. Karpitschka, H. Riegler, *Langmuir* 26, 11823 (2010).

[3] S. Karpitschka, H. Riegler, *PRL* 109, 066103 (2012).

CPP 44.9 Thu 17:45 H39

Droplet morphologies in a cylindrical tube — ●CIRO SEMPREGON, STEPHAN HERMINGHAUS, and MARTIN BRINMANN — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Equilibrium conformations of droplets on cylindrical fibers and their transitions during changes of volume and contact angle have been studied for almost a century. Liquid morphologies in a tube, however, have received only little attraction. Here, we present the results of a combined analytical and numerical study of droplet shapes wetting the inside of a cylinder at zero buoyancy. For any contact angle the liquid forms a plug bounded by two spherical surfaces if the volume is sufficiently large. In the opposite limit of small volumes, the liquid interface adopts the shape of a spherical cap which is slightly deformed by the curved surface. At intermediate volumes and small contact angle an annular morphology is observed which can be described as the analog to the barrel droplet on a fiber. In contrast to the barrel droplets the mechanical stability of this morphology is limited by the appearance of either an axisymmetric or a non-axisymmetric soft mode. Stability with respect to the latter type of mode can be related to the existence of an inflection point in the droplet contour as already demonstrated for barrel droplets [1]. Based on our findings a complete morphology diagram is constructed in terms of contact angle and volume.

[1] H B Eral et al.: "Drops on functional fibers: from barrels to clamshells and back" *Soft Matter* 7 (2011) 5138

CPP 44.10 Thu 18:00 H39

Dynamics of Immiscible Fluid Flow through Porous Media

— ●KAMALJIT SINGH^{1,2,3}, HAGEN SCHOLL³, ALEN KABDENOV^{2,3}, MARCO DI MICHIEL¹, MARIO SCHEEL¹, STEPHAN HERMINGHAUS², and RALF SEEMANN^{2,3} — ¹European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble, France — ²Max Planck Institute for Dynamics and Self-Organization, D-37073 Goettingen, Germany — ³Saarland University, Experimental Physics, D-66041 Saarbruecken, Germany

The pore-scale dynamic behavior of water imbibition into an initially oil filled porous medium was investigated in situ using synchrotron X-ray tomography. We investigated the effect of various factors, including wettability, viscosity and density of fluids, flow velocity and pore structure, on the quantitative and qualitative behaviour of the fronts. The findings reveal that for low capillary numbers the water-oil front behavior is independent of all other factors except for wettability. The wettability decides the nature of the front and the final oil saturation after a complete water flood. The front is more compact for small contact angles of the imbibing water phase. This compact front results in almost no oil trapping after a complete flood. However, the front roughens with increasing contact angle and progresses in elongated capillary fingers for large contact angles. The formation of fingers results in significant oil trapping (10-15%).

CPP 44.11 Thu 18:15 H39

Imbibition of electrolytes into nanoporous gold and electrocapillary effects

— ●YAHUI XUE^{1,2}, JÜRGEN MARKMANN^{1,3}, PATRICK HUBER³, HUILING DUAN², and JÖRG WEISSMÜLLER^{1,3} — ¹Helmholtz-Zentrum Geesthacht, Institut für Werkstofforschung, Werkstoffmechanik, 21502 Geesthacht, Germany — ²State Key Laboratory for Turbulence and Complex System, Department of Mechanics and Aerospace Engineering, College of Engineering, Peking University, Beijing 100871, China — ³Technische Universität Hamburg-Harburg, Institut für Werkstoffphysik und -technologie, 21073 Hamburg, Germany

Electrocapillary techniques exhibit great advantages in nonmechanical electrofluidic manipulation, e.g., flow actuation in micro-/nanochannels. One issue of interest is the spontaneous imbibition of fluids in bodies with a nanoscale pores size. Contrary to previous studies we here use a metallic nanoporous body. This allows us to control the electrode potential at the solid-fluid interface. Nanoporous gold (NPG) with uniform pore- and ligament size of ~ 45 nm was fabricated by dealloying an Ag₇₅Au₂₅ alloy. Spontaneous imbibition of aqueous electrolytes obeys the Lucas-Washburn law. Electrocapillary effects were then used to manipulate the imbibition dynamics. Due to the enhanced wetting, the Washburn law predicts an acceleration of the imbibition by $\sim 60\%$. Yet, imbibition experiments show only $\sim 25\%$ acceleration. A possible explanation is that the ion transport capability through nanopores limits the charging of the double layer at the invasion front, which is confirmed by potential step coulometry experiments.

CPP 44.12 Thu 18:30 H39

Microfluidics of ordered fluids — ●ANUPAM SENGUPTA, CHRISTIAN BAHR, and STEPHAN HERMINGHAUS — Max Planck Institute for Dynamics and Self Organization, Am Fassberg 17, 37077 Göttingen

Flow of ordered fluids (e.g. liquid crystals) is inherently complex due to the coupling between the flow and the long-range orientational order. Experiments carried out at micro scales further reveal the influence of surface properties on the static and dynamic outcomes. We use microfluidics as a platform to tune one or more of the above competing components, and explore the resulting equilibrium states. The delicate but intricate balance between the viscous, elastic and surface forces was consequently used to devise opto-fluidic and micro-scale-transport applications. On one hand the novel applications complement the conventional microfluidic capabilities, and on the other hand, broaden the reach of 'isotropic' microfluidics by offering competitive advantages. Standard microfluidic techniques and a combination of polarizing optical microscopy, fluorescence confocal polarizing microscopy and particle tracking methods were employed for the investigations.

[1] Nematic textures in microfluidic environment by A. Sengupta, U. Tkalec, Ch. Bahr, *Soft Matter* 7, 6542, 2011.

[2] Functionalization of microfluidic devices for investigation of liquid crystal flows by A. Sengupta, B. Schulz, E. Ouskova, Ch. Bahr, *Microfluidics and Nanofluidics*, DOI: 10.1007/s10404-012-1014-7, 2012.

[3] Opto-fluidic velocimetry using liquid crystal microfluidics by A. Sengupta, S. Herminghaus, Ch. Bahr, *Applied Physics Letters* 101, 164101, 2012.

CPP 45: Colloids and Complex Liquids II

Time: Thursday 15:00–18:45

Location: H40

Invited Talk

CPP 45.1 Thu 15:00 H40

Interacting colloidal fluids self-assembled from supramolecular polymers — TINGZI YAN¹, KLAUS SCHRÖTER¹, FLORIAN HERBST², WOLFGANG BINDER², and •THOMAS THURN-ALBRECHT¹ — ¹Institute of Physics, Martin-Luther University Halle-Wittenberg — ²Institute of Chemistry, Martin-Luther University Halle-Wittenberg

It is well established that small or medium sized molecules carrying groups with specific interactions can form supramolecular polymers and networks. In many cases, the specificity of the underlying interactions is most prominent in dilute solution. We present a supramolecular system based on polyisobutylene polymers with thymine and 2,6-diaminotriazine functional end groups forming well-defined micellar aggregates in the melt whose properties can be described as that of an interacting colloidal fluid. The concentration of micelles depends on temperature leading to a solid-fluid ordering transition for monofunctional polymers which shows up in structure as well as in the rheological properties. Bifunctional polymers on the other hand can form hydrogen-bonds between micelles leading to a temperature dependent solidification by gelation without ordering.

CPP 45.2 Thu 15:30 H40

New particle-to-mesh scheme for modeling high-molecular weight dense polymer systems — •GUOJIE ZHANG¹, KOSTAS CH. DAOULAS^{1,2}, and KURT KREMER¹ — ¹Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany — ²Innovation Lab GmbH, Speyerer Straße 4, 69115 Heidelberg, Germany

We consider a recently proposed model of high-molecular weight polymeric systems representing the molecules by chains of soft spheres with fluctuating size. Within this description, we develop a grid-based Monte Carlo method for efficient modeling of polymer melts. The soft spheres represent Gaussian density distributions of segments of underlying microscopic sub-chains. The coordinates and the radii of the spheres are defined in continuum space and simple bonded potentials keep the chain connectivity. The non-bonded interactions are defined via a discretized functional of the local density, obtained by mapping the density clouds of the spheres onto a grid, without requiring a neighbor list. The accuracy of the method is verified by comparing the results of the grid-based simulations with data obtained from a standard potential-based description. In contrast to most lattice-based descriptions, the approach allows for simulations in the isothermal-isobaric ensemble. Subsequently, the perspectives of the new scheme for creating equilibrated configurations of long polymer melts with microscopic level of detail are discussed. For this purpose, we introduce a hierarchical strategy increasing gradually the resolution of the model.

CPP 45.3 Thu 15:45 H40

Clustering in β -lactoglobulin and lysozyme protein solutions studied by SAXS — •BO JING¹, FAJUN ZHANG¹, FELIX ROOSEN-RUNGE¹, MICHAEL SZTUCKI², and FRANK SCHREIBER¹ — ¹Institute of Applied Physics, University of Tübingen — ²ESRF, Grenoble, France

The understanding of protein cluster formation provides insight into protein function, crystallization and protein aggregation induced diseases. β -lactoglobulin (BLG) is known to form dimers, tetramers, hexamers and octamers at certain pH, temperature, and salt concentrations. Here, we present SAXS measurements which indicate oligomer formation at high protein concentrations, in the absence of salt and other additives. Scattering curves of BLG solutions display a major correlation peak which shifts minimally to higher q -values with increasing protein concentration. This observation is indicative of cluster formation or, in this case, oligomerization. We draw a comparison with the well-studied lysozyme protein system, where we observed a more pronounced shift of the major correlation peak that has been associated with the formation of a dynamical cluster phase. In this system, the peak position also shows a temperature dependence not seen with BLG solutions. The SAXS data of both systems were fitted to elliptical form factors and two-Yukawa interaction potentials. We relate the different clustering models and contrasting temperature responses in these protein systems to differences in their interaction potential and the distinct properties of BLG and lysozyme proteins molecules. In this context, the shortcomings of isotropic interaction models and the

need to consider patchy interactions are also discussed.

CPP 45.4 Thu 16:00 H40

Finding Colloidal Hard Spheres — MARKUS FRANKE¹, ACHIM LEDERER¹, SEBASTIAN GOLDE¹, ECKHARD BARTSCH², and •HANS JOACHIM SCHÖPE^{1,3} — ¹Johannes Gutenberg Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Germany — ²Albert-Ludwigs-Universität Freiburg, Institut für Physikalische Chemie, Albertstr. 21, 79104 Freiburg — ³Max-Planck-Institut für Polymerforschung, Postfach 3148, 55021 Mainz, Germany

In two recent publications it was claimed that there are difficulties in the preparation and characterization of colloids with hard sphere (HS) like interaction [1, 2]. Using PMMA-PHSA particles dispersed in organic solvents serious deviations from the ideal HS behavior have been observed. Furthermore the authors are of the opinion that in general the experimental determination of the particle volume fraction suffers from an inaccuracy of 0.03 to 0.06. Using highly cross linked polystyrene particles dispersed in ethylnaphtalene an optical and gravity matched colloidal model system with HS like interaction can be realized. We performed a comprehensive characterization of our colloidal model system giving us the possibility to determine the particle volume fraction with an accuracy better than 0.01. Analyzing different physical properties (sedimentation velocity, equilibrium phase behavior, crystallization kinetics, equilibrium lattice constant, glass transition dynamics, collective diffusion, short time diffusion) over a large volume fraction range (0.01 up to 0.74) we can show that this particles monitor HS behavior over the entire concentration range. [1] *Soft Matter* 8, 21 (2012), [2] *Soft Matter* 9, 17 (2013)

CPP 45.5 Thu 16:15 H40

How elasticity influences the dynamics of bead-spring-chains in shear flow — •JOHANNES GREBER and WALTER ZIMMERMANN — LS Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth

Simulations of dumbbells in shear flow show that in the semi-diluted regime of a dumbbell suspension individual dumbbells make flips after unpredictable time intervals [1].

With the help of the Fluid Particle Dynamics (FPD) we simulate suspensions of flexible dumbbells corresponding to high Weissenberg numbers Wi and low Reynolds numbers Re [2,3]. We investigate how the flexibility of springs connecting the two beads of a dumbbell (measured by Wi) influences the mixing behaviour in a dumbbell suspension. Further we compare the dynamics of the flow of a dumbbell suspension with the turbulent flow regime in Newtonian fluids at high Reynolds numbers.

References

- [1] J. Bammert et al. (preprint)
- [2] H. Tanaka and T. Araki, *Phys. Rev. Lett.* 85, 1338 (2000)
- [3] P. Peyla, *EPL* 80, 34001 (2007)

CPP 45.6 Thu 16:30 H40

Shear-induced diffusion of spheroidal particles in non-Brownian suspensions at low Reynolds numbers — •FLORIAN JANOSCHEK, FEDERICO TOSCHI, and JENS HARTING — Eindhoven University of Technology, Eindhoven, The Netherlands

Hydrodynamic diffusion can strongly enhance mass and heat transport in microfluidic systems. However, while several authors discussed the shear-induced self-diffusion of spherical particles in experiment, theory, and simulation at low or vanishing Reynolds numbers, less is known about the case of non-spherical particles that are present in suspensions as different as blood, mud, or paint. We present our numerical study of concentrated suspensions of rigid particles at different oblate and prolate aspect ratios. The hydrodynamic self-diffusion is compared with the one obtained for spherical particles and the effect of asphericity at varying volume fractions is discussed.

15 min break

CPP 45.7 Thu 17:00 H40

Gold Nano Rods Close to Charged and Uncharged Surfaces: Slowing Down of Rotational and Translational Diffusion — •MARYAM HAGHIGHI¹, MUHAMMAD NAWAZ TAHIR², WOLFGANG TREMEL², HANS-JÜRGEN BUTT¹, and WERNER STEFFEN¹ —

¹Max Planck Institute for Polymer Research, P.O. Box 3148, 55128 Mainz, Germany — ²Institut für Anorganische Chemie und Analytische Chemie der Johannes Gutenberg-Universität, Duesbergweg 10-14, D-55099 Mainz, Germany

Diffusion and rotation of gold nanorods close to a solid interface were studied with two recently introduced techniques: Resonance Enhanced Dynamic Light Scattering (1) and Waveguide Enhanced Dynamic Light Scattering (2). We observed strong, plasmon-enhanced light scattering. Gold nano rods were stabilized by cetyltrimethylammonium bromide (CTAB). They showed an unexpected strong slowing down of the translational diffusion coefficient, whereas for rotational diffusion this slowing down is distinct but less pronounced. To find the possible influence of charges on the solid interface on this slowing we varied the added salt concentration. Another approach was to cover the metal interface with an electrically neutral layer of poly-methylmethacrylate. A third approach was to completely exchange CTAB for its covalently bound, thiolated analogue 16-mercaptohexadecyl trimethylammonium bromide (MTAB), this reduces the slowing down considerably. (1) Plum MA, Menges B, Fytas G, Butt HJ, Steffen W, Rev. Sci Instr. 2011, 82, 015102 (2) Plum MA, Vianna SDB, Unger A, Roskamp RF, Butt HJ, Menges B, Steffen W, Soft Matter 2011, 7, 1501

CPP 45.8 Thu 17:15 H40

Phase behavior of colloidal monolayers on one-dimensional periodic light potentials — ●LAMISS ZAIDOUNY, THOMAS BOHLEIN, and CLEMENS BECHINGER — 2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany

Phase transitions of colloidal monolayers on light-induced substrate potentials have been demonstrated to provide novel insights into the phase behavior of two-dimensional systems on patterned surfaces. Due to the interplay of repulsive inter-particle forces and their interaction with the substrate, interesting structures will form which are also observed in atomic systems. Here, we study the phase transitions of charged colloidal particles on arrays composed of periodic one-dimensional laser lines which are created by a scanned laser beam. The colloidal particles used are suspended in an organic solvent with low polarity that causes the formation of spontaneous hexagonal crystals of large lattice constants as compared to those formed in aqueous solutions. This fact provided a new regime where phase transitions are accessed for different periods of the light patterned substrates.

CPP 45.9 Thu 17:30 H40

Percolation thresholds and critical exponents of colloidal suspensions in bulk and confinement — ●HELGE NEITSCH and SABINE H. L. KLAPP — Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

We performed extensive grand canonical Monte Carlo simulations to investigate the percolation transition of spherical colloids a) in the bulk phase and b) confined between two parallel, chemical undecorated walls (slit pore) [1]. The interaction between the colloids is modeled through a square-well potential with an attraction range of only 4% of the hard core diameter to mimic the ultra-short ranged nature of depletion attractions [2]. Applying a finite-size analysis, we investigated the density threshold of the connectedness percolation at several wall separations (width of the slit pore). Increasing the wall separation, we found a shift of the percolation threshold towards the bulk value obtained from an unconfined, in other respects identical system. We could explain this shift by scaling arguments, which are usually applied in the framework of cross-over scaling of the vapor-liquid critical point of simple liquids in slit pores [3]. In addition we studied the critical exponents of the percolation transition and found them to be remarkably insensitive to the width of the slit pore.

- [1] H. Neitsch and S. H. L. Klapp, submitted, arXiv:1211.1027 (2012)
 [2] P. J. Lu, E. Zaccarelli, F. Ciulla, A. B. Schofield, F. Sciortino, and D. A. Weitz, Nature **453**, 499 (2008)
 [3] R. L. C. Vink, K. Binder, and J. Horbach, Phys. Rev. E **73**, 056118 (2006)

CPP 45.10 Thu 17:45 H40

Confinement induced repulsion in oscillatory structural forces — ●SEBASTIAN SCHÖN and REGINE VON KLITZING — Stranski-Laboratorium, Department of Chemistry, TU Berlin, Straße des 17. Juni 124, D-10623 Berlin

Suspensions of nanoparticles show a layered ordering in the vicinity of surfaces. Overlap of these regions, as under confinement conditions,

leads to oscillatory changes in the ordering behavior of the particles, dependent on the exact wall to wall distance. These changes originate from the entropic excluded volume effect and indicate a break in the translational symmetry of the bulk system.

Force measurements have been performed by Colloidal Probe Atomic Force Microscopy (CP-AFM), where the colloidal probe on the cantilever and the substrate act as confining surfaces. Forces can be extracted from the deflection signal of the cantilever and are normalized with the radius of the colloidal probe to get the corresponding force curves. These provide a direct means to the structural response of the nanoparticles during a gradual change of the confinement.

Investigation of suspensions with varying ionic strength and pH, invoked via addition of sodiumchloride, sodiumhydroxide or hydrochloric acid, show an additional repulsion underlying the normal structural force signal as described by Israelachvili. The key parameters of the oscillatory force signal, namely amplitude, wavelength and decay-length as well as the extra repulsion are compared for suspensions with different additives.

CPP 45.11 Thu 18:00 H40

Phase transitions and phase equilibria in spherical confinement — ●ANTONIA STATT, ALEXANDER WINKLER, PETER VIRNAU, and KURT BINDER — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany

The interplay of finite size and surface effects for fluids confined in a sphere is studied via Monte Carlo simulations of the Asakura-Oosawa model for colloid-polymer mixtures¹ using free energy calculations. For this model the phase separation in a colloid-rich phase and a polymer-rich phase is well known in the bulk^{2,3} and we show that spherical confinement enhances the miscibility of the mixture. Depending on the wall potentials of the confining surface, the wetting properties can be controlled, and this interplay between adsorption of one species to the confining surface and bulk unmixing leads to very special shapes of the loops observed for the chemical potential of the colloids.

- [1] S. Asakura and F. Oosawa, J. Polym. Sci. **33**, 183
 [2] R.L.C. Vink and J. Horbach, J. Chem. Phys. **121**, 3253
 [3] R.L.C. Vink, J. Horbach, and K. Binder, Phys. Rev. E **71**,011401

CPP 45.12 Thu 18:15 H40

Fluids in extreme confinement — ●THOMAS FRANOSCH¹, SIMON LANG¹, and ROLF SCHILLING² — ¹Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058, Erlangen, Germany — ²Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany

For extremely confined fluids with two-dimensional density n in slit geometry of accessible width L , we prove that in the limit $L \rightarrow 0$ the lateral and transversal degrees of freedom decouple, and the latter become ideal-gas-like [1]. For small wall separation the transverse degrees of freedom can be integrated out and renormalize the interaction potential. We identify nL^2 as hidden smallness parameter of the confinement problem and evaluate the effective two-body potential analytically, which allows calculating the leading correction to the free energy exactly. Explicitly, we map a fluid of hard spheres in extreme confinement onto a 2d-fluid of disks with an effective hard-core diameter and a soft boundary layer [1]. Two-dimensional phase transitions are robust and the transition point experiences a shift $O(nL^2)$.

- [1] Thomas Franosch, Simon Lang, and Rolf Schilling, Phys. Rev. Letter (2012) in press

CPP 45.13 Thu 18:30 H40

Coarse-graining strategies for coronene molecules — ●THOMAS HEINEMANN and SABINE H. L. KLAPP — Institut für theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin

Coarse-graining describes the idea of systematically integrating out irrelevant degrees of freedom in order to create an effective Hamiltonian, which allows to investigate larger length- and time scales. In this contribution we focus on the coarse-graining of coronene molecules from atomistic detail to mesoscopic molecular detail. So far only a complicated, temperature-independent coarse-grained model for coronene, used for static calculations, exists [1].

A hierarchy of model potentials generating different many-particle aspects of coronene, e.g. crystal stability, aggregation, etc., will be introduced. These models are studied via mesoscopic Molecular Dynamics simulations. As a basic platform for molecular pair interactions, the Gay-Berne potential with electric multipoles (GBEMP), which has been established [2], is used. This ansatz is combined with param-

eters characterizing the electronic contributions as well as shape contributions from atomistic, biased Umbrella Sampling simulations. The fitting procedure of the models will be discussed.

- [1] O. I. Obolensky et al., *Int. J. Quantum Chem.* 107 (2007) 1335.
 [2] P. Xu et al., *J. Mol. Model.* (2012), doi:10.1007/s00894-012-1562-5.

CPP 46: Photovoltaics (joint session HL/CPP/O)

Time: Friday 9:15–13:45

Location: H2

CPP 46.1 Fri 9:15 H2

Simulation of TRPL on thin film solar cells — ●MATTHIAS MAIBERG, MARIA GAUDIG, and ROLAND SCHEER — Institute of Physics, Martin-Luther-University Halle-Wittenberg, Von-Danckelmann-Platz 3, 06406 Halle, Germany

In the recent years time-resolved photoluminescence (short: TRPL) on semiconductor devices has been established as a non-destructive, non-invasive, contactless characterization method. The decay of the signal has not been fully understood yet. Therefore we studied TRPL on semiconductor layers and thin film solar cells by simulation with Synopsys TCAD. At first we investigated the influence of excitation, diffusion, photon recycling, bulk-defects and defects at the contacts, as well as space charge and potential fluctuations on the PL-decay separately by quasi-one-dimensional simulations of absorber layers and thin film solar cells. We also studied the influence of grain boundaries, since materials like $\text{Cu}(\text{In,Ga})\text{Se}_2$ and $\text{Cu}_2\text{ZnSnSe}_4$ are in general polycrystalline. We show, that the samples can be characterized by excitation dependent measurements in the open circuit case. We can explain some effects found in photoluminescence experiments, like a decrease of the lifetime with an increasing excitation, a maximum lifetime due to saturated bulk-defects, and a lifetime of more than $10\mu\text{s}$ in case of charge separation due to the electric field in the space charge region.

CPP 46.2 Fri 9:30 H2

3D reciprocal space imaging of individual $\text{Cu}(\text{In,Ga})\text{Se}_2$ nanocrystallites inside a thin film solar cell — ●TARAS SLOBODSKYY¹, ANATOLIY SLOBODSKYY², BORIS LANDGRAF¹, CHRISTIAN HEYN¹, and WOLFGANG HANSEN¹ — ¹Institute for Applied Physics, University of Hamburg, Jungiusstraße 11, D-20355 Hamburg, Germany — ²Karlsruhe Institute of Technology (KIT), Light Technology Institute (LTI), Kaiserstraße 12, 76131 Karlsruhe, Germany

In this contribution we will present results of an investigation of strain distributions inside of individual $\text{Cu}(\text{In,Ga})\text{Se}_2$ nanocrystallites located inside a solar cell absorber layer. The strain is imaged using synchrotron radiation.

We find that the investigated crystallites are non homogeneously strained. The strain is produced by surrounding nanocrystals in the polycrystalline semiconductor film and carries information about the intercrystalline interactions. The measurements are done non destructively and without additional sample preparation or X-ray beam nanofocusing.

The demonstrated technique provides a way for connecting variations in the properties of individual crystallites inside of a working solar cell to the resulting energy conversion efficiency.

CPP 46.3 Fri 9:45 H2

Investigations of chemical gradients in $\text{Cu}(\text{In,Ga})\text{Se}_2$ thin film solar cells grown on polyimide substrate by high spatially resolved cathodoluminescence microscopy — ●STEFAN RIBBE^{1,2}, ANDREAS RAHM¹, FRANK BERTRAM², and JÜRGEN CHRISTEN² — ¹Solarion AG, Ostende 5, 04288 Leipzig, Germany — ²Institute for Experimental Physics, Otto-von-Guericke-Universität Magdeburg, Germany

Optical properties of $\text{Cu}(\text{In,Ga})\text{S}_2$ (CIGS)-absorber layers for thin film solar cells have been studied by high spatially resolved cathodoluminescence (CL) at low temperature ($T = 5\text{K}$) to investigate lateral and vertical changes of the composition within the quaternary absorber. CIGS layers were grown on flexible polyimide foil by using an ion-beam assisted roll-to-roll process. To ensure high efficiency sodium fluoride was evaporated by an additional source during the process. The substrate temperature was varied above the standard value enabled by using an advanced polyimide substrate resisting higher temperatures. Cross sections of the thin film solar cells were prepared to investigate the vertical distribution of composition and its changes influenced by the substrate temperature. IV measurements showed an increase of

the efficiency with higher substrate temperature suggesting less fluctuation of the composition and a smoother vertical gallium gradient. Furthermore a variation of the sodium content was made by variation of the evaporation temperature. Integral luminescence properties were investigated which showed a red shift and a broadening of the main peak with increased sodium content.

CPP 46.4 Fri 10:00 H2

Admittance spectroscopy on $\text{Cu}(\text{In,Ga})\text{Se}_2$ solar cells with respect to sodium content — ●FELIX DAUME^{1,2}, ANDREAS RAHM¹, and MARIUS GRUNDMANN² — ¹Solarion AG, Ostende 5, 04288 Leipzig, Germany — ²Institut für Experimentelle Physik II, Universität Leipzig, Linnéstraße 5, 04103 Leipzig, Germany

Solar cells based on $\text{Cu}(\text{In,Ga})\text{Se}_2$ (CIGSe) absorbers deposited on flexible polyimide substrate enable cheap manufacturing with roll-to-roll equipment and the application in new environments such as low-load rooftops. Among present thin film flexible solar cell technologies, CIGSe achieves the highest efficiencies. The proper incorporation of sodium into the CIGSe absorber is indispensable to achieve these high efficiencies. In this study, sodium fluoride is co-evaporated during CIGSe deposition.

CIGSe solar cells with different sodium contents were investigated by admittance spectroscopy. We calculated activation energies for the N1 signature which, in literature, is widely attributed to defects. Overall concentrations and density profiles across the band gap were derived for this signature. Additionally, we derived the net doping of the CIGSe absorbers from capacitance-voltage measurements. A model based on defects at the $\text{CdS}(\text{n-type})/\text{CIGSe}(\text{p-type})$ interface is proposed to explain our observations with respect to the sodium content.

CPP 46.5 Fri 10:15 H2

High-resolution Spectroscopic Mapping of Polymer Fullerene Blend Films for Organic Solar-Cell Applications — XIAO WANG, KAI BRAUN, ALFRED J. MEIXNER, and ●DAI ZHANG — Institute of Physical and Theoretical Chemistry, Uni. Tübingen, Tübingen

Polymers and fullerenes are widely employed in the field of organic solar cells as the electronic donors and acceptors. The morphology and the photo-physical properties of the polymer and fullerene blends at nanometer scale are critical for achieving a high performance of the solar cells. Employing a home-built parabolic mirror assisted apertureless near-field optical (Raman and photoluminescence) microscope, we demonstrated high resolution near-field spectroscopic mappings of the polymer:fullerene blend films. Our investigation focused on the additive effect for a C-PCPDTBT:PCBM blend film. From the simultaneously recorded morphology and spectroscopic information, the interplay among the blend film morphology, the local donor and acceptor molecular distributions, and the photoluminescence quenching efficiency were discussed. The PL and Raman signals of the electron donor and acceptor have been probed at an optical resolution of approximately 10 nm which allow the direct identification of the chemical nature of the different domains. Moreover, we were able to reveal and quantify the local quenching, which is related to the electron transfer from donor to acceptor.

CPP 46.6 Fri 10:30 H2

Investigation of the s-shape caused by the hole selective layer in organic bulk heterojunction solar cells — ●LOTHAR SIMS^{1,2}, ULRICH HÖRMANN², RENÉ KOGLER³, ROLAND STEIM⁴, WOLFGANG BRÜTTING², and PAVEL SCHILINSKY¹ — ¹Belectric OPV GmbH, Landgrabenstr. 94, 90443 Nürnberg — ²University of Augsburg, Institute of Physics, Universitätsstr. 1, 86135 Augsburg — ³Evonik Industries AG, Kirschenallee, 64293 Darmstadt — ⁴STORM Energy GmbH, Rathenauplatz 2, 90489 Nürnberg

During the operation period of an organic solar cell different failure mechanisms can occur which limit the lifetime of the device. Among these failure mechanisms the so called s-shape or second diode, where the current density-voltage (JV) curve bends towards the origin in the

4th quadrant, plays an important role. We investigated the origin of the s-shape caused by the hole selective layer (HSL) using N,N'-bis(3-methylphenyl)-N,N'-bis(phenyl)-benzidine (TPD) coevaporated with different amounts of Dipyrazino[2,3-f:2',3'-h]quinoxaline-2,3,6,7,10,11-hexacarbonitrile (HATCN) as a model system. The low glass transition temperature of TPD allows investigating the impact of WF and mobility of the HSL on device performance and thus s-shape independently of each other. The observed JV-curves were simulated by solving the drift-diffusion, i.e. continuity and Poisson equations numerical via the program PC1D. While WF rather influences the open circuit voltage, mobility seems to be the reason for the s-shape. The results show that an accumulation of holes near the hole selective/semiconductor layer interface might be responsible for the observed s-shape.

CPP 46.7 Fri 10:45 H2

The role of defects in nanocrystalline zinc oxide interlayers for polymer-based solar cells — ●SEBASTIAN WILKEN, DOROTHEA SCHEUNEMANN, FLORIAN WITT, JÜRGEN PARISI, and HOLGER BORCHERT — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, Carl-von-Ossietzky-Str. 9-11, 26129 Oldenburg, Germany

In polymer-based bulk heterojunction solar cells, the absorber blend has intrinsically no preferential transport direction for photogenerated charge carriers due to the statistical intermixing of both the donor and acceptor phase. Therefore, additional charge-selective interfacial layers, which are semipermeable membranes for either electrons or holes in an ideal case, are widely used in order to achieve efficient charge extraction at the respective contacts. One well established material for electron collection is zinc oxide (ZnO), which can be processed at moderate temperatures and deposited via solution-based techniques in form of colloidal nanocrystals (NCs). Here, we discuss the influence of defect states in interlayers made of ZnO NCs on the overall solar cell performance. For that purpose, ZnO NCs with different surface-to-volume ratios were wet-chemically synthesized and introduced into indium tin oxide-free polymer solar cells in the inverted device architecture. As indicated by photoluminescence, we show that surface defects play a more and more dominant role with decreasing NC size and, thus, limit the photovoltaic efficiency. For a more detailed analysis of the involved defect states, photo-induced current transient spectroscopy (PICTS) was performed for devices with varying amount of surface defects.

CPP 46.8 Fri 11:00 H2

Solar diode sensor — ●HAO SHEN¹, MARTIN HOFFMANN¹, JUAN DANIEL PRADES², FRANCISCO HERNANDEZ-RAMIREZ³, and ANDREAS WAAG¹ — ¹Institute of Semiconductor Technology, TU Braunschweig, D-38105 Braunschweig, Germany — ²Department of Electronics, Uni. Barcelona, E-08028 Barcelona, Spain — ³Catalonia Institute for Energy Research (IREC), E-08930 Barcelona, Spain

The nanodevice architecture presented here has been designed to overcome the current issues in gas sensor technologies: reducing power consumption and lowering operating temperature. Conductometric sensors based on semiconductor metal oxides need the continuous supply of the energy in the form of heat or UV light, to activate the chemical interaction between gases and the sensing surface. New concepts for energy harvesting units as an in-built module are demanded to make self-powered gas sensors. Herein we report a solar diode sensor (SDS) based on new designed CdS@n-ZnO/p-Si nanoelements which unifies gas sensing (CdS@n-ZnO) and solar energy harvesting (n-ZnO/p-Si diode) functionalities in a singular material unit and device. The SDS sensing mechanism (change of open circuit voltage), in comparison to the well-known conductometric sensors (change of resistance), is systematically studied and explained in terms of gas-material surface interactions and the subsequent changes in the doping level (ND), which is manifested in the variation of Voc in CdS@n-ZnO/p-Si. The fabricated SDS was capable of quantitatively detecting oxidising and reducing gases with reproducible response at room temperature and without the need of any other energy sources except solar illumination.

CPP 46.9 Fri 11:15 H2

Simulation of temperature distribution in ZnO:Al thin films for laser annealing experiments — ●CHRISTIAN ISENBERG, CAY-CHRISTIAN KALMBACH, DANİYAL SATTARIAN, UWE STUTE, and ALEXANDER HORN — Laser Zentrum Hannover e.V., Hollerithallee 8, 30419 Hannover, Germany

Transparent Conducting Oxides (TCOs) have become widespread as transparent electrodes in photovoltaics and transparent electronics.

Thermal post deposition treatments by furnace annealing have shown to improve the electrical and optical properties of TCO thin films. Laser annealing of TCOs allows control over the peak temperature as well as the spatial and temporal temperature distributions of TCO thin films and substrates, preserving the substrate by heating only the TCO layer. Therefore, treating TCOs with tailored laser radiation allows larger temperature than furnace annealing even on temperature sensitive substrates. Numerical calculations using Crank-Nicolson method have been conducted to estimate the temperature distribution in ZnO:Al thin films during laser annealing process. In the special case of temperature-independent material parameters, the numerical solution is reduced to an analytical solution, determined by convolution of the heating source term with a Green's function for a geometry of a thin film on a semi-infinite substrate. Numerical results are compared to temperature measurements, done by a thermographic camera during laser annealing process.

Coffee break

CPP 46.10 Fri 11:45 H2

Selective laser ablation of Al₂O₃ passivation layers from optically black silicon surfaces — ●MARTIN OTTO¹, KATHARINA WIDDER¹, TINO RUBBLACK¹, MATTHIAS ZILK², THOMAS KÄSEBIER², GERHARD SEIFERT¹, and RALF B. WEHRSPORN³ — ¹Martin-Luther-University Halle-Wittenberg, Institute of Physics -μ MD Group, Heinrich-Damerow-Strasse 4, 06120 Halle, Germany — ²Friedrich Schiller University Jena, Institute of Applied Physics, Max-Wien-Platz 1, 07743 Jena, Germany — ³Fraunhofer Institute for Mechanics of Materials Halle, Walter-Hülse-Str. 1, 06120 Halle, Germany

Inductive coupled plasma reactive ion etching (ICP-RIE) of silicon enables excellent broad band and wide angle antireflective surface properties. The stochastically emerging needle like nano-structures let the silicon surface appear optically black due to its high absorption coefficient of over 97% integrated from 300 nm to 1175 nm. Concomitant, highly enhanced surface recombination is introduced. The latter, may be effectively suppressed by a well suited passivation layer of Al₂O₃ deposited by thermal ALD. Laser ablation is commonly used in the PV industry to open local contact areas in dielectric passivation stacks. In this work we show the feasibility to ablate alumina thin films from nano-structured black silicon (b-Si) solar cell front surfaces. Microstructural geometric analysis by focussed ion beam and SEM reveal certain structural changes in the zone of ablation which are believed to be beneficial for contact formation. Simultaneously, neither the deposition of Al₂O₃ layers of varying thickness nor their ablation lead to a very significant degradation of the optical surface properties.

CPP 46.11 Fri 12:00 H2

Surface Modification of Nano-Textured Black Silicon for Photovoltaic Applications — ●MICHAEL ALGASINGER¹, SVETOSLAV KOYNOV¹, JULIE PAYE¹, FLORIAN WERNER², MAX BERT¹, MARTIN S. BRANDT¹, and MARTIN STUTZMANN¹ — ¹Walter Schottky Institut, Technische Universität München, 85748 Garching, Germany — ²Institute for Solar Energy Research Hamelin, Am Ohrberg 1, 31860 Emmerthal, Germany

The morphology and the electronic properties of nano-textured silicon, obtained by a metal-catalyzed wet etching process and its improvement by an additional chemical treatment are examined with regard to solar cell applications. Photoluminescence and optical reflectivity measurements show evidence for a nano-porous silicon (np-Si) phase in the as-prepared nanostructure. It is found that an additional wet-chemical treatment removes the np-Si fraction and significantly alters the surface of the nanostructure. Cross-sectional scanning electron microscopy images reveal a drastic reduction of the surface area, to values of only 3 - 6 times of that of a planar surface. Electron spin resonance measurements were performed to investigate the type and quantity of defects induced by the nano-texturing process. First results on the passivation of surface defects via atomic layer deposition of Al₂O₃ are presented. Photoconductance decay measurements of passivated nanostructures, which received the additional post-etching treatment, show a significant increase in effective carrier lifetimes.

CPP 46.12 Fri 12:15 H2

Surface morphology of black silicon produced by metal-catalyzed wet etching — ●MAXIMILIAN BERT, MICHAEL ALGASINGER, SVETOSLAV KOYNOV, and MARTIN STUTZMANN — Walter Schottky Institut, Technische Universität München, 85748 Garching, Germany

Nano-textured silicon, also referred to as black silicon (b-Si), is a material with an optically graded surface, which shows reflectivity as low as 1 - 5 % in the whole range of Si absorption and additional light trapping effects. Due to its unique optical properties, b-Si is an interesting material for photovoltaic applications. However, b-Si produced by Au-catalyzed wet etching of crystalline Si (c-Si) wafers exhibits a nano-porous silicon (np-Si) phase in the as-prepared nano-structure. This np-Si phase leads to an increased surface area which could alter the electrical properties significantly. The formation of the nano-texture was investigated at different stages of the etch process by cross sectional scanning electron microscopy. The evolution of the np-Si phase with increasing etch time was observed by photoluminescence and optical reflectivity measurements. In addition, the influence of the doping level of n- and p-type c-Si substrates on the etch process and the morphology of the resulting nano-texture was studied.

CPP 46.13 Fri 12:30 H2

Valence band offsets estimation of Al₂O₃ films on silicon by XPS and UPS measurements — ●JOHANNES ZIEGLER¹, VOLKER NAUMANN², MARTIN OTTO¹, ALEXANDER SPRAFKE¹, and RALF B. WEHRSPORN^{1,3} — ¹Martin-Luther-University Halle-Wittenberg, Institute of Physics, Halle, Germany — ²Fraunhofer Center for Silicon Photovoltaics CSP,Halle, Germany — ³Fraunhofer Institute for Mechanics of Materials Halle, Halle, Germany

A quantitative measurement of valence band offsets in isolator-silicon junctions might help to realize heterojunction devices such like semiconductor-isolator-semiconductor (SIS) solar cells. We measured XPS and UPS spectra of thin (2–50 nm thick) Al₂O₃ films deposited on silicon by thermal ALD. The valence band offsets of these structures are estimated from the XPS spectra using the method of Kraut et.al. [1]. A slight trend in the valence band offsets 3.3–4.5 eV with increasing film thickness 2–50 nm was calculated from the XPS spectra. To estimate the valence band offsets from the UPS spectra 3.3–3.4 eV of 2–10 nm thick Al₂O₃ on silicon, a simple straight forward approach based on linear regression of the spectra on the band edges is used. We compare the results of both measurements and discuss possible sources for the measured increase of the valence band offset with increasing Al₂O₃ film thickness.

[1] A. Kraut, R. W. Grant, J. R. Waldrop and S. P. Kowalczyk, Phys. Rev. Lett. 44,p.1620 (1982), <http://link.aps.org/doi/10.1103/PhysRevLett.44.1620>

CPP 46.14 Fri 12:45 H2

Charge trapping in Al₂O₃ passivation layers for silicon solar cells — ●PAUL JORDAN¹, FRANK BENNER¹, INGO DIRNSTORFER¹, and THOMAS MIKOLAJICK^{1,2} — ¹NaMLab gGmbH, Dresden, Germany — ²Lehrstuhl für Nanoelektronische Materialien, TU Dresden, Dresden, Germany

Novel highly efficient silicon solar cells require an excellent level of surface passivation, to minimize recombination losses of photo-generated carriers. During the last decade, the dielectric Al₂O₃ became the material of choice for the passivation of p-type silicon. The excellent passivation properties are mainly caused by negative charges located within the dielectric. In this study the origin of the negative charges is investigated using capacitance-voltage and microwave detected photo-conductivity measurements. It will be shown that the negative charges are partly caused by electrons, injected from silicon into the dielectric. The trapping dynamics are analyzed by the means of the post program discharge technique, which is commonly applied for memory devices. Furthermore, the trapping and detrapping rates depend on the thickness of the ultra-thin SiO₂ interface between Si and Al₂O₃. For an

interface thickness of about 2 nm, the asymmetry of trapping and detrapping rates significantly enhances the negative charge density. As a consequence an optimum interface thickness is essential for the excellent passivation property of Al₂O₃.

CPP 46.15 Fri 13:00 H2

Investigation of carrier traps in pn-junctions of fully-processed silicon photovoltaic cells — ●TEIMURAZ MCHEDLIDZE, LEOPOLD SCHEFFLER, and JÖRG WEBER — Technische Universität Dresden, 01062 Dresden, Germany

Mesa-diodes with a surface area about 1 mm² and a height of 50 μm were fabricated on top of fully-processed Si photovoltaic-cell wafers for detection and investigation of carrier traps in pn-junctions. All fabrication steps were performed at room temperature and fully preserved the initial structure of the cell inside the mesa-diode. Schottky diodes were fabricated on neighbor locations of the wafers after etching off the PV-cell structure to a depth of 50 μm. The DLTS spectra detected for the mesa- and Schottky-diodes show significant difference, namely the deep carrier traps detected in the mesa-structures were below the detection limit in the Schottky-diodes. Profiling of the trap density for the mesa-diodes showed a steep decrease with increasing distance from the pn-junction. Parameters of the detected traps, their possible origin and reasons for the differences between spectra detected for mesa- and Schottky-diodes are presented and discussed.

CPP 46.16 Fri 13:15 H2

Iron acceptor association in compensated multicrystalline silicon — ●CHRISTIAN MÖLLER^{1,2}, KEVIN LAUER¹, FABIEN GIBAJA³, TIL BARTEL³, and FRITZ KIRSCHT³ — ¹CiS Forschungsinstitut für Mikrosensorik und Photovoltaik GmbH, SolarZentrum Erfurt, Konrad-Zuse-Str. 14, 99099 Erfurt, Germany — ²TU Ilmenau, Institut für Physik, Weimarer Str. 32, 98693 Ilmenau, Germany — ³Calisolar GmbH, Magnusstraße 11, 12489 Berlin

Monitoring the acceptor concentration in compensated multicrystalline silicon by a minority-charge carrier lifetime measurement is applicable for production control due to the fast and easy lifetime measurement. The iron acceptor pair association is studied for several acceptors position dependent over the whole height of a compensated multicrystalline ingot. Acceptor pair and height dependent induced differences in the defect kinetics are visible. The calculated position depending doping concentrations of several ingots from charge carrier lifetime measurements are discussed and compared with the expected doping concentration calculated via Scheil equation.

CPP 46.17 Fri 13:30 H2

Femtosecond laser processed sulfur-emitter solar cells — ●THOMAS GIMPEL¹, KAY-MICHAEL GÜNTHER², ANNA LENA BAUMANN¹, WOLFGANG SCHADE¹, and STEFAN KONTERMANN¹ — ¹Fraunhofer Heinrich Hertz Institute, EnergieCampus, Am Stollen 19B, 38640 Goslar, Germany — ²Energieforschungszentrum Niedersachsen, EnergieCampus, Am Stollen 19B, 38640 Goslar, Germany

A simple fs-laser process enables structuring and sulfur incorporation simultaneously. This process is applied on a single side to different silicon substrates independent from the crystal structure. Without any advanced solar engineer processes like passivation, dopant source layer deposition, its diffusion and removal, efficiencies of 8.2% are achieved, at present. Due to an incorporated intermediate band this material has the potential to convert infrared light even at wavelengths below the silicon band gap. New applications e.g. in a crystalline silicon tandem solar cell are under development.

CPP 47: Charged Soft Matter

Time: Friday 9:30–12:00

Location: H34

Invited Talk

CPP 47.1 Fri 9:30 H34

Ion transport in polyelectrolyte materials: Mechanisms and general scaling concepts — ●MONIKA SCHÖNHOF, CORNELIA CRAMER, SOUVIK DE, and AMRTHA BHIDE — University of Münster, Münster, Germany

Polyelectrolyte multilayers (PEM) and polyelectrolyte complexes (PEC) are interesting materials for application as ion conductors, as they can be tuned with defined thickness or defined stoichiometry, re-

spectively. Ac conductivity spectra characterize the ionic transport processes over many decades of frequency, providing a full picture of long-range as well as local motions. In temperature-dependent spectra of dry PEC the time-temperature superposition principle (TTSP) is shown to be valid. For spectra taken at different relative humidity a new scaling principle in analogy to TTSP termed time-humidity superposition principle is established. This model-free scaling holds for different materials over several decades in frequency. It implies that the hydration is activating ion motion over short and long distances

in a similar general way, a concept so far only established for thermal energy.

CPP 47.2 Fri 10:00 H34

Single molecule investigation of complexes of oppositely charged bottle brushes — ●IVAN RAGUZIN^{1,2}, GEORGI STOYCHEV^{1,2}, and LEONID IONOV¹ — ¹Leibniz-IPF Dresden, 01069 Dresden, Germany — ²TU Dresden, 01062 Dresden, Germany

We experimentally investigated complexation of oppositely charged bottle polymer brushes at the single-molecule level using AFM and CryoTEM. It was found that polyelectrolyte complexes have "scrambled-egg" morphology where oppositely charged polymer chains are not oriented parallel to each other but are intercrossed. Moreover, we observed that in CryoTEM polymer chains in IPEC appear brighter compared to the background that is in contrast to darker polymer chains of the individual components. We believe that the reason for this effect is the release of counter ions of the polymer brushes due to the neutralization of the charged side groups of the polymer chains [1].

[1] Soft Matter, 2013, Advance Article

CPP 47.3 Fri 10:15 H34

Substrate Dominated versus Bulk Phase Dominated Polyelectrolyte Multilayer: The Swelling Effect — ●MAXIMILIAN ZERBALL and REGINE VON KLITZING — Institute of Chemistry, Stranski-Laboratorium, TU Berlin, 10623 Berlin, Str. 17.Juni 124

For the past twenty years, the Layer-by-Layer technique (LbL) has made it possible to modify surfaces by covering them with thin films. This technique gives the opportunity for a wide variety of potential applications for polyelectrolyte multilayers (PEM), for example chemical reactors, antireflective coatings or microcontainers. For all these applications, it is from greatest interest to control thickness and structure of the film perfectly. Additionally it is important to know how external stimuli change the film properties.

The thickness, more precisely the distance of the film/air interface away from the substrate influences the structure of the film. For the initial layers the structure is mainly influenced by the chemical nature of the substrate. After a certain number of layers the effect of the substrate vanishes completely and the PEM properties are mainly dominated by the bulk behavior of the polyelectrolyte system. Further, these structure changes influencing the swelling behavior of the PEM.

This study is focusing on the correlation between the structure and the swelling behavior of PEM in these two different regimes. For that purpose, the properties of the PEM are monitored after the deposition as a function of the number of layers by Ellipsometry, Atomic Force Microscopy and X-Ray Reflectometry under different relative humidity.

CPP 47.4 Fri 10:30 H34

Self assembly of block copolymer films in confined geometries, electric fields and epitaxy. — ●ULRICH WELLING and MARCUS MÜLLER — Institut für theoretische Physik, Friedrich-Hund Platz 1, 37075 Göttingen

Strategies for controlling the orientation and defect density in self-assembled structures of copolymers have attracted abiding interest. Using Single-Chain-in-Mean-Field Monte-Carlo simulations we study the influence of inhomogeneous electric fields on the self-assembled morphologies of symmetric, lamella-forming copolymer. We present results on the influence of electric fields and the effect of solved ions on the ordering kinetics in thin films and on chemically patterned substrates.

CPP 47.5 Fri 10:45 H34

Rotational and translational diffusion of ionic liquids confined in nanoporous silica — ●CIPRIAN GHIORGHITA IACOB, JOSHUA SANGORO, WYCLIFFE KIPNUSU, JÖRG KÄRGER, and FRIEDRICH KREMER — Institute of Experimental Physics I, Leipzig, Germany

Charge transport and glassy dynamics of several classes of ionic liquids confined in uni-directional nanoporous silica membranes are investigated in a wide frequency and temperature range by a combination of Broadband Dielectric Spectroscopy (BDS), Pulsed Field Gradient Nuclear Magnetic Resonance (PFG NMR) and Fourier Transform Infrared spectroscopy (FTIR). Two opposite effects are observed: (i) surface effects and (ii) confinement effects. More than 10-fold systematic decrease in the effective diffusion coefficient (for HMI+ -based ionic

liquids with PF6⁻, I⁻, Cl⁻, Br⁻ anions) from the bulk value is observed in the silica nanopores. For a second category of ILs including BF4⁻ and NTF2⁻-based ionic liquids, it is experimentally demonstrated that the ionic mobility at lower temperatures is enhanced by more than two decades under nano-confinement in comparison to the bulk value. In summary, the resultant macroscopic transport properties of glass-forming ionic liquids in confining space are determined by a subtle interplay between surface- and confinement- effects [1-4].

References: [1]. Iacob, C., (2008) J. Chem. Phys., 129 (23) 234511, [2]. Iacob, C., et al. (2010). Phys. Chem. Chem. Phys., 12, 13798-13803, [3]. Iacob, C., et al. (2011). Soft Matter, 8, 289-293, [4]. Kremer, F., Schönhals, A.,(2003) Broadband Dielectric Spectroscopy, Berlin: Springer.

CPP 47.6 Fri 11:00 H34

Understanding microscopic processes in ionic liquids via MD-simulations — ●VOLKER LESCH and ANDREAS HEUER — Westfälische Wilhelms-Universität Münster, Münster, Germany

Ionic liquids are promising candidates for electrolyte applications. One disadvantage is the slow lithium diffusion so improvements related to this property would be very useful. To investigate such transport processes, we employ MD-simulations as a powerful tool for a microscopic analysis.

Here we compare the properties of bis(fluorosulfonyl)imide (FSI) and bis(trifluoromethylsulfonyl)imide (TFSI). Although both anions are quite similar their properties are surprisingly different. More specifically, our research consists out of two parts. First, we study systems with the same counterion for lithium and EMIM. Many research groups only work on these systems because they cover different voltage ranges. In our investigations we focus on dynamical and structural properties. As one would expect the dynamics of the system which contains TFSI is much slower. This is related to stronger bonds between TFSI and lithium ions and an enhanced viscosity due to the sterical demands of TFSI. Second, we analyzed systems with mixed anions (ratio 1:0.29). These systems combine the properties of the two anions but unfortunately the electrochemical stability window decreases. Especially, the effects of FSI on TFSI and vice versa are of particular interest. Increasing the amount of TFSI leads to a faster dynamic for TFSI and slower dynamics for FSI. This contrasts to the results for the systems with the same counterion for both cations.

CPP 47.7 Fri 11:15 H34

Impedance spectroscopy of ions at liquid-liquid interfaces — ●ANDREAS REINDL, MARKUS BIER, and S. DIETRICH — Max Planck Institute IS, Stuttgart, Germany, and University of Stuttgart, Germany

We consider theoretically the dynamics of the ions in electrolytic cells with liquid-liquid interfaces by using dynamic density functional theory. This approach leads to a generalized Nernst-Planck equation the solutions of which are used to determine the experimentally accessible quantities impedance and dielectricity. We could find alternative circuits consisting only of the classic components ohmic resistance and capacitance which approximate the calculated spectra very well. Supported by the circuits, statements about the ion dynamics at the interface are possible for all frequencies.

CPP 47.8 Fri 11:30 H34

An ionic force field optimization approach: single- and ion-pair thermodynamic properties — ●MARIA FYTA^{1,2} and ROLAND NETZ^{2,3} — ¹Institut für Computerphysik, Universität Stuttgart, Germany — ²Department Physik, Technische Universität München, Germany — ³Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany

We propose a novel approach to derive well optimized classical ionic force fields. For this optimization we include single-ion as well as ion-pair thermodynamic properties simultaneously. Our newly optimized force fields for different halide and alkali ions are derived in conjunction to the SPC/E water model at finite ion concentration. We first fix ion-water parameters based on single-ion solvation free energies, and in a second step determine the cation-anion interaction parameters (traditionally given by the mixing rules). From the finite-concentration simulations, thermodynamic properties, such as the osmotic coefficients of the salt solutions are calculated and compared to relevant experimental data. For the size-symmetric salt solutions involving bromide and chloride ions, this scheme using the standard mixing rules works fine, but not for the iodide and fluoride solutions, which correspond to the largest and smallest anion we have considered and require a

rescaling of the mixing rules. Our results show that for iodide, the experimental activities suggest more tightly bound ion pairing than given by the standard mixing rules. For fluoride, the simulations show a large attraction between fluoride and cations. We finally, discuss the transferability of the proposed ionic force fields.

CPP 47.9 Fri 11:45 H34

Why ions promote first-order wetting — •INGRID IBAGON, MARKUS BIER, and S. DIETRICH — Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany

Wetting studies of electrolyte solutions have shown that electrostatic

interactions promote first order wetting transitions [1,2,3]. In this work we present an analytic expression of the effective interface potential within a model for an electrolyte solution near a charged wall, which is derived from an expansion of the density functional around a sharp kink density profile [4]. The analysis enables us to draw an intuitive picture of the conditions under which the presence of ions will promote first-order wetting.

[1] N. A. Denesyuk and J.-P. Hansen, *J. Chem. Phys.* 121, 3613 (2004).

[2] A. Oleksy and J.-P. Hansen, *Mol. Phys.* 107, 2609 (2009).

[3] I. Ibagon, M. Bier, and S. Dietrich, in preparation.

[4] I. Ibagon, M. Bier, and S. Dietrich, in preparation.

CPP 48: (Hydro)gels and Elastomers

Time: Friday 9:30–12:00

Location: H39

Invited Talk

CPP 48.1 Fri 9:30 H39

The distribution of segmental order in polymer networks — •MICHAEL LANG¹ and JENS-UWE SOMMER^{1,2} — ¹Leibniz Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden — ²Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden

The monomer fluctuations and the distribution of segmental order is derived for a slip tube model of polymer entanglements assuming random walk statistics of the tube sections [M. Lang, J.-U. Sommer, *Physical Review Letters* 104 (2010) 177801]. The predictions are compared with simulation data of model networks that were created using the bond fluctuation method. The comparison reveals that local fluctuations of the tube statistics do not affect the distribution function as averaged over the full sample. Instead, length fluctuations of the confining tube control the shape of the distribution function. Furthermore, a narrowing of the distribution function is determined, if the cross-linking occurs on the time scale of the relaxation of the network strands. Almost instantaneously cross-linked poly-disperse samples do not show this narrowing and are well described by tube length fluctuations that agree to previous work on the dynamics of melts of star polymers. The difference between the stress optical law and the time average segment orientations is discussed and our results are compared to previous simulation studies in literature.

CPP 48.2 Fri 10:00 H39

Local chain deformation and stress distributions in strained elastomers — MARIA OTT¹, ROBERTO PÉREZ-APARICIO², HORST SCHNEIDER¹, PAUL SOTTA², and •KAY SAALWÄCHTER¹ — ¹Institut für Physik-NMR, Martin-Luther-Univ. Halle-Wittenberg, Betty-Heimann-Str. 7, D-06120 Halle, Germany — ²Laboratoire Polymères et Matériaux Avancés, CNRS/Rhodia, Saint Fons, France

Macroscopic strain applied to elastomeric networks induces changes in the orientation fluctuations of the chain segments [1]. This effect can be used to study the local stretching of elastically active chains by suitable NMR methods [2]. Importantly, the method also reveals inhomogeneities, i.e., distributions in local stress, which is particular relevant for elastomers filled with (nano)particles. We have studied a series of natural rubber samples with different cross-link densities and amounts of filler particles. The data is incompatible with predictions of the well-established affine-Gaussian model [3], but can be reproduced on the basis of more recent treatments of the local deformation based upon the tube and phantom models. For the first time, we demonstrate the existence of matrix overstrain in commercially relevant filled elastomers in agreement with simple hydrodynamic predictions.

[1] J.-U. Sommer et al., *Phys. Rev. E* 78, 051803 (2008)

[2] K. Saalwächter, *Prog. Nucl. Magn. Reson.* 51, 1-35 (2007)

[3] P. Sotta, B. Deloche, *Macromolecules* 23, 1999-2007 (1990)

CPP 48.3 Fri 10:15 H39

Elastic properties of squeezed spheres made of superabsorbers — •THOMAS JOHN and CHRISTIAN WAGNER — Experimentalphysik, Universität des Saarlandes

Superabsorbent polymers may absorb pure water up to 500 times its weight. Granulates of mm size can swell up to perfect spheres with up to 20 mm in diameter. The perfect spherical symmetry may be a combination of surface tension and inner pressure. Compressing of the spheres between two plates yields a force-strain relation. We present

a model to calculate this force strain relation. The model conserves the volume and the restoring force is caused by the change of surface area made from the deformation. This is opposite to the Hertzian theory in contact mechanics, within the elastic modulus of the material plays the important role. Our model calculations are compared with experimental obtained force-strain data.

[1] Lu, W.-M. et al, *Powder Technology* 116, 1, (2001). [2] Lin, Y.-L. et al, *Chemical Engineering Science* 63, 195, (2008).

CPP 48.4 Fri 10:30 H39

Investigation of a multiresponsive hydrogel based on poly(methoxydiethylenglycol acrylate) (PMDEGA) with azobenzene moieties — •DAVID MAGERL¹, DAVID EGGER¹, ANNA MIASNIKOVA², ANDRÉ LASCHEWSKY², CHRISTINE M. PAPADAKIS¹, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department, Lehrstuhl Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany — ²Institut für Chemie, Universität Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam-Golm, Germany

Stimuli-responsive hydrogels are of increasing interest because of their use in a variety of applications such as drug-delivery and sensors. In this context hydrogels that are responsive to one external stimulus like temperature, as it is the case for poly(methoxydiethylenglycol acrylate) (PMDEGA), are widely studied. [1] By addition of moieties of azobenzene groups to form a statistical copolymer, a second stimulus, namely light, can be added to the system.

In this study we are investigating in the complex interplay between the temperature and light sensitive properties in the P(MDEGA-stat-azoMDEGA) system with varied azoMDEGA content. Dynamic light scattering is used to probe the hydrodynamic radius in aqueous solutions. On the other hand, white light interferometry gives access to the time-resolved swelling behavior in thin films at the presence of a water vapor atmosphere.

[1] Zhong, Q., et al., *Soft Matter*, 2012. 8(19): p. 5241-5249.

CPP 48.5 Fri 10:45 H39

Evaluation of Fluorophore-Functionalized Thermoresponsive Copolymers for Sensor Applications — •SAHIKA INAL¹, JONAS D. KÖLSCH², LEONARDO CHIAPPISI³, DIETMAR JANIEZ⁴, MICHAEL GRADZIELSKI³, ANDRÉ LASCHEWSKY², and DIETER NEHER¹ — ¹Inst. of Physics and Astronomy, Univ. of Potsdam, Germany — ²Dept. of Chemistry, Univ. of Potsdam, Germany — ³Stranski-Laboratory, Dept. of Chemistry, TU Berlin, Germany — ⁴Fraunhofer Inst. for Applied Polymer Research, Potsdam, Germany

Water-soluble polymers respond to changes in solution temperature by altering their conformation [1]. Although the fundamental mechanisms leading to these solubility transitions are comparable for the most studied LCST-type polymers, e.g., poly(N-isopropylacrylamide) (pNIPAm) and oligo(ethylene glycol) methacrylate (OEGMA) based copolymers, each type of polymer backbone has a peculiar solvation behavior and experiences different changes in the micro-environment upon phase transition. Here, we investigate the solubility transition behavior of NIPAm- and OEGMA-based copolymers bearing a dye-functionalized comonomer through their temperature-dependent photophysical properties. With the polarity-sensitive dye incorporated to the side chains, the emission spectra of these copolymers are expected to undergo similar changes upon phase transition. However, the two dye-labeled polymers exhibit rather different fluorescence responses, pointing to particular solvation properties of acryl amide and ethylene

oxide based polymers, and rendering them useful for different sensing strategies. [1] V. O. Aseyev et al., *Adv. Polym. Sci.* 2006, 196, 85.

CPP 48.6 Fri 11:00 H39

Immobilization of water soluble peroxidase within p-NIPAM microgel particles for the usage in organic solvents — ●KORNELIA GAWLITZA¹, RADOSTINA GEORGIEVA², and REGINE VON KLITZING¹ — ¹Stranski-Laboratorium, Institut für Chemie, Technische Universität Berlin — ²Charité Universitätsmedizin Berlin, Department of Enzyme Technology

Enzymes are of high research interest in the field of catalysis. To reach a high stability in the presence of organic solvents, enzymes can be immobilized within a polymer matrix. Microgel particles made of poly-*N*-isopropylacrylamide (p-NIPAM) are promising as polymer matrix due to their reversible shrinking above the volume phase transition temperature (VPTT). In this study, large p-NIPAM microgels with a cross-linker content of 0.25% were synthesized via surfactant free emulsion polymerization using a temperature ramp[1]. The polymer particles were characterized by Dynamic Light Scattering (DLS) and Atomic Force Microscopy (AFM). Afterwards, water soluble peroxidase was immobilized within the polymer network using a solvent exchange from polar to organic solvents[2],[3]. The immobilized system shows an enhanced activity in isopropanol and the localization of the enzymes has been proven by confocal laser scanning microscopy (CLSM). [1] Meng, Z.; Smith, M. H.; Lyon, L. A. *Colloid. Polym. Sci.* 2009, 287, 277. [2] Gawlitza, K.; Wu, C.; Georgieva, R.; Wang, D.; Ansoerge-Schumacher, M.-B.; Klitzing, v. R. *Phys. Chem. Chem. Phys.* 2012, 14, 9594. [3] Gawlitza, K.; Wu, C.; Georgieva, R.; Ansoerge-Schumacher, M.-B.; Klitzing, v. R. *Z. Phys. Chem.* 2012, 226, 749

CPP 48.7 Fri 11:15 H39

Mechanical properties of magneto-sensitive elastomers: microscopic theory versus continuum-mechanics approach — ●DMYTRO IVANEYKO^{1,2}, VLADIMIR TOSHCHEVIKOV², MARINA SAPHIANNIKOVA², and GERT HEINRICH^{1,2} — ¹Technische Universität Dresden — ²Leibniz-Institut für Polymerforschung Dresden e.V.

We compare predictions of continuum-mechanics approach and our microscopic theory [1,2] for the mechanical behaviour of magneto-sensitive elastomers (MSEs) under a uniform external magnetic field. The continuum-mechanics approach is based on the calculation of deformation-dependent demagnetization factor and predicts the elongation of MSEs. The microscopic theory explicitly considers the point-like dipole interactions between magnetic particles and gives a different sign of the magnetostriction depending on the spatial distribution of particles [1,2]. Also, the sample shape plays an essential role in the mechanical properties of MSEs. We show that the microscopic theory predicts the same results as continuum-mechanics approach in the case of ellipsoidal MSE samples with isotropic particle distributions. Moreover, the values of demagnetization factor are found to be the same for stochastic and isotropic lattice distributions. They change however considerably for chain-like particle distributions. Generalization of the continuum-mechanics approach for the case of anisotropic particle distributions is currently in progress.

[1] D. Ivaneiko et al., *Macromolecular Theory and Simulations* 20,

411 (2011).

[2] D. Ivaneiko et al., *Condensed Matter Physics* 15, 33601(2012).

CPP 48.8 Fri 11:30 H39

Computer Simulations of Magnetic Gels — ●RUDOLF WEEBER¹, SOFIA KANTOROVICH^{2,3}, and CHRISTIAN HOLM¹ — ¹Institut fuer Computerphysik, Universitaet Stuttgart, Allmandring 3a, 70569 Stuttgart — ²Sapienza, University of Rome, Iazza A. Miro 5, 00185 Italy — ³Ural Federal University, Lenin Av. 51, Ekatarinburg, 620083 Russia

Magnetic gels consist of magnetic nano-particles embedded in a cross-linked polymer network. They have potential applications ranging from medicine to engineering, e.g., drug release systems and artificial muscles. These applications rely on the combination of the mechanical properties of the polymer network with the ability to modify and control the sample with external magnetic fields due to the embedded magnetic nano-particles.

Today, many aspects of the synthesis of ferrogels are understood and the properties of gels can be characterized and tailored. However, many questions concerning the microstructure and its influence on macroscopic properties of magnetic gels are still open. Here computer simulations can help since they allow to study simplified model systems which focus on certain characteristic features of the material.

In this contribution we present a computer model for a gel, which is cross-linked by magnetic nano-particles. When the nano-particles orient to align to an external field, they drag the polymer chains attached to them and thereby deform the gel. In the presentation, we will explore the deformation mechanism in two and three dimensions as well as the elastic properties of the system.

CPP 48.9 Fri 11:45 H39

Large-strain detection using elastomeric sensors — ●TINA MEISSNER, MATTHIAS KOLLOSCH, and REIMUND GERHARD — Universität Potsdam, Institut für Physik und Astronomie, Potsdam, Germany

Electroactive polymers (EAP) and soft stretchable conductors have been studied extensively to develop voltage-tunable dielectric elastomer actuators (DEA) that can achieve large deformations at low voltage. However, the advantages of this DEA technology can also be used for strain-sensing solutions. While conventional strain sensors, e.g. made of piezoelectric materials, are limited to strains not exceeding 2 to 3% due to their mechanical properties, elastomeric sensors are able to detect both small and large strains, up to 300%. Furthermore, they offer the advantages of high sensitivity in the low-stress regime, fast response times, low power consumption, and good weathering stability.

The proposed capacitive strain sensor consists of a dielectric elastomer film sandwiched between highly stretchable polymeric electrodes. Its functional principle is based upon the coupling between mechanical deformations and changes in the sensor's capacitance. We present experimental strategies to enable large reversible mechanical deformations as well as the use of ceramic/polymer nano-composites and molecular composites to adjust strain sensitivity and durability. One potential application is demonstrated on large-scale experiments: the sensor serving as a diagnostic tool for the structural health of infrastructural facilities.

CPP 49: Colloids and Complex Liquids III

Time: Friday 9:30–12:00

Location: H40

Invited Talk

CPP 49.1 Fri 9:30 H40

Interface-controlled property adjustment in ionic liquid/inorganic hybrid materials — ●ANDREAS TAUBERT — University of Potsdam

Ionic liquids (ILs) have classically been used as solvents, for extraction, and catalysis. Materials synthesis and the adjustment of the properties of IL/inorganic and IL/polymer hybrid materials (ionogels) by tuning the interaction between an IL and the host material have recently attracted growing interest.

The advantage of ILs is that, by virtue of the large number of available IL components, their properties such as ionic conductivity or phase behavior can be adjusted.

Among others, IL-based hybrid materials are attractive candidates, for example, as membranes in fuel cells or batteries, in hybrid magnetic

materials, or in multiresponsive materials. In order to understand, control, adapt, and extend the application of ionogels, the parameters controlling the structure, thermodynamics, phase behavior, and transport properties within the ionogels must be known.

The presentation will highlight some recent approaches towards quantification of these and other properties and highlight new developments towards transport of protons and ions in these highly complex nanostructured materials that could be of relevance for, e.g., energy research.

CPP 49.2 Fri 10:00 H40

In situ high pressure XPS for ionic liquid - gas phase reaction studies — ●INGA NIEDERMAIER¹, WEI WEI², CHRISTIAN PAPP¹, CLAUDIA KOLBECK¹, SANDRA KRICK CALDERÓN¹, FLORIAN MAIER¹, PETER SCHULZ², PETER WASSERSCHIED², and HANS-PETER

STEINRÜCK¹ — ¹Lehrstuhl für Physikalische Chemie II — ²Lehrstuhl für Chemische Reaktionstechnik, Egerlandstr. 3, 91058 Erlangen

Ionic liquids (ILs) are molten salts composed solely of ions with a melting point below 100 °C and a negligible vapour pressure at room temperature. X-ray photoelectron spectroscopy (XPS) has proven to be a versatile tool for surface investigations of these materials under ultrahigh vacuum conditions (UHV).^[1] It even allows to monitor reactions occurring in the near-surface region of ILs.^[2] We demonstrate to our knowledge the first gas-liquid reaction studies between an IL and a gaseous species by means of *in situ* XPS in the mbar pressure regime. The anion of the IL $[\text{Me}_2\text{N}^+(\text{CH}_2\text{CH}_2\text{OH})_2][\text{H}_2\text{NCH}_2\text{CH}_2\text{SO}_3^-]$ was functionalised with an amine group (H_2N^-), in analogy to aqueous amine systems for carbon dioxide capture applications. ILs are considered as potential replacements for these aqueous amines due to the extremely low vapour pressure and their typically high thermal stability. Under CO_2 pressures up to 0.9 mbar, *in situ* XPS reveals reaction schemes involving carbamate and ammonium formation via carbamic acid as an intermediate. Supported by the Cluster of Excellence - Engineering of Advanced Materials. 1. H. P. Steinrück, Phys Chem Chem Phys, **2012**, 14, 5010 2. I. Niedermaier et al., Chemphyschem, **2012**, 13, 1725

CPP 49.3 Fri 10:15 H40

Self Assembly in a Magnetic Room Temperature Ionic Liquid (MRTIL) — ●ANDREAS KLEE¹, SYLVAIN PREVOST^{1,2}, and MICHAEL GRADZIELSKI¹ — ¹Stranski Laboratorium für Physikalische und Theoretische Chemie, TU Berlin, Straße des 17. Juni 124, 10623 Berlin, Germany — ²Helmholtz-Zentrum Berlin für Materialien und Energie, Glienicker Straße 100, 14109 Berlin, Germany

Magnetic room-temperature ionic liquids (MRTIL) are a specific class of RTIL where an ion confers a magnetic susceptibility to the liquid, which in turn exhibits a paramagnetic behavior. The first occurrence of this new class of liquid media was discovered in 2004 [1, 2] based on the organic cation 1-butyl-3-methylimidazolium (bmim^+) and the anion tetrachloroferrate (FeCl_4^-). Thanks to the high spin FeCl_4^- , a small magnet is enough to modify the meniscus of the fluid, and stronger macroscopic effects are visible when the surface tension is reduced. MRTIL can be used as a solvent for self assembly of surfactant systems which leads to structures like micelles, liquid crystals, macro- and microemulsions including magnetic properties [3]. New insights into the nature of self assembly by studying these water-free, aprotic systems are expected. [1] S. Hayashi and H. O. Hamaguchi, *Chem. Lett.*, **33**, 1590-1591, (2004) [2] S. Hayashi et al., *IEEE Trans. Magn.*, **42**, 12-14, (2006) [3] A. Klee, S. Prevost, W. Kunz, R. Schweins, K. Kiefer, M. Gradzielski, *Phys. Chem. Chem. Phys.*, **14**, 15355-15360, (2012)

CPP 49.4 Fri 10:30 H40

Magneto-optical measurement of the rotational relaxation of nickel nanorod colloidal dispersions in ac magnetic fields — ●MICA GRATZ, ANDREAS TSCHÖPE, and RAINER BIRRINGER — Universität des Saarlandes, Saarbrücken, Deutschland

The dynamical magnetic and magneto-optical response of nickel nanorod colloidal dispersions in ac magnetic fields was investigated. The nanorods with an average diameter of ≈ 25 nm and an average length of ≈ 200 nm, were prepared by pulsed electrodeposition of nickel into nanoporous AA0-templates. Dissolution of the alumina layer in dilute NaOH with polyvinylpyrrolidone (PVP) for steric stabilization followed by separation and purification resulted in a stable aqueous dispersion of the nanorods. The microstructure of the nanorods was characterized by electron microscopy and the magnetic properties were obtained from static magnetization measurements and field-dependent optical transmission of linearly polarized light. Furthermore, the rotational relaxation in ac magnetic fields was investigated by ac-magnetization and ac-magneto-optical transmission measurements. The experimental results were analyzed by comparison with numerical solutions of the Fokker-Planck equation of rotational diffusion in ac magnetic fields to derive the characteristic relaxation time of the nanorods.

CPP 49.5 Fri 10:45 H40

Systems of magnetic anisotropic particles: microstructure and macroproperties — ●ELENA PYANZINA¹ and SOFIA KANTOROVICH^{1,2} — ¹Ural Federal University, Lenin av. 51, 620000, Ekaterinburg, Russia — ²Sapienza, University of Rome, Piazza A. Moro 5, 00185, Rome, Italy

Anisotropic particles form the cutting edge of dipolar soft matter research as they correspond completely to the idea of fine tuning and designing new materials with controllable properties. In this contribution we present a theoretical study and computer simulations of the microstructure and macroproperties of magnetic ellipsoids and cylinders. As the first step, the analysis of the possible ground state structures (the most energetically favoured configurations at 0 K) for two and three dimensions is carried out. Then, we propose a method of calculating analytically the pair correlation function for the combination of Gay-Berne and magnetic dipole-dipole potential based on the group integral technique. An extensive comparison of the theoretical model and the results of molecular dynamics simulations for different semi-axes ratios demonstrated a very good agreement for two and three dimensions for both types of the particles. We conclude, that even slight shape anisotropy can lead to the drastic change in the microstructure and, as a result in macroscopic responses of the system. Changing the asphericity of particles and their density both the ground states and the equilibrium room temperature properties can be tuned and effectively controlled.

CPP 49.6 Fri 11:00 H40

Colloidal particles at liquid interfaces — ●JENS HARTING, STEFAN FRIJTERS, and FLORIAN GÜNTHER — Department of Applied Physics, Eindhoven University of Technology, Den Dolech 2, 5600MB Eindhoven

Emulsions stabilized by particles are ubiquitous in the food and cosmetics industry, but our understanding of the influence of microscopic fluid-particle and particle-particle interactions on the macroscopic rheology is still limited. Modern simulation algorithms based on a multi-component lattice Boltzmann model to describe the solvents combined with a molecular dynamics solver for the description of the suspended particles allow to tune the particle size, shape, wettability and surface tensions between the fluids.

We report on the adsorption of spherical or ellipsoidal particles to liquid interfaces and demonstrate the existence of stable and semi-stable equilibrium states. On larger scales, different phases of stabilized emulsions have been found. While Pickering emulsions are already known for more than a century, so-called bicontinuous interfacially jammed emulsion gels (Bijels) were only predicted recently. The particles can fully arrest domain growth and a transition between both phases can be found by tuning the concentration, contact angle, or fluid ratio. Further, by tuning the particle shape additional geometrical degrees of freedom add additional time scales to the arrest of domain growth.

CPP 49.7 Fri 11:15 H40

SANS study of polymer loaded microemulsions — ●ANDREAS WEBER¹, HENRICH FRIELINGHAUS², and BERND STÜHN¹ — ¹Experimental Condensed Matter Physics, TU Darmstadt, Germany — ²Jülich Centre for Neutron Science, Germany

The interactions between polymers and soft surfactant layers are subject of current research interest. We study these interactions in microemulsions in the droplet phase, where surfactant stabilized droplets of water are dispersed in a matrix of octane. Small angle neutron scattering experiments allowed us to observe directly the effect of a polymer on an anionic or non-ionic surfactant layer. To microemulsion droplets of different sizes composed by either AOT or C_{12}E_4 we added different amounts of the hydrophilic polymer PEG. While matrix and water core of the microemulsion were deuterated, the surfactant and polymer were protonated, thus, allowing us to observe the surfactant shell influenced by the polymer. We observe, as predicted by theory and indirect measurements such as dielectric spectroscopy, that the polymer interacts differently with a nonionic or an anionic surfactant shell: Apart from an increase of polydispersity of the droplets in both cases, in the former case the addition of polymer seems not to affect the surfactant shell. In the latter case, the obtained scattering data show that the anionic surfactant layer is strongly influenced. We develop a model describing the scattering of the polymer inside the polymer loaded droplet and fit it to the data. The obtained results are compared to small angle x-ray scattering, dynamic light scattering and dielectric spectroscopy experiments on this system done in our group.

CPP 49.8 Fri 11:30 H40

Bilayer undulation dynamics in unilamellar phospholipid vesicles: Influence of temperature, cholesterol and trehalose — ●BEATE-ANNETTE BRÜNING¹, SYLVAIN PRÉVOST^{1,2}, RALF STEHLE¹, ROLAND STEITZ¹, PETER FALUS³, BELA FARAGO³, and THOMAS HELLWEG⁴ — ¹Helmholtz Zentrum Berlin, Hahn-Meitner

Platz 1, 14109 Berlin, Germany — ²Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany — ³Institut Laue-Langevin, B. P. 156, 38042 Grenoble Cedex 9, France — ⁴Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany

We report a combined dynamic light scattering (DLS) and neutron spin-echo (NSE) study on lipid vesicles composed of 1,2-dimyristoyl-sn-glycero-3-phosphatidylcholine (DMPC), respectively under the influence of temperature and the membrane additives cholesterol and trehalose. We study bilayer undulation and bulk diffusion dynamics using neutron spin-echo spectroscopy, on two distinct time scales, namely around 25 ns and 100 ns. Finally, we calculate the respective bilayer bending rigidities κ for all types of lipid vesicles. We observe a bilayer softening around the main phase transition temperature T_m of the single lipid model system, and a bilayer stiffening the more cholesterol is added, whereas the insertion of trehalose hardly changes the bilayer undulations and membrane rigidity κ [1]. We explain our findings on the basis of a free volume available to lipid molecules in the membrane plane, which encounters the most pronounced changes in the acyl chain regime. [1] B. Brüning, S. Prévost, R. Stehle, R. Steitz, P. Falus, B. Farago, T. Hellweg, submitted.

CPP 49.9 Fri 11:45 H40

Shaping of Unilamellar Vesicles by the Admixture of Am-

phiphilic Copolymer — •MICHAEL GRADZIELSKI¹, KATHARINA BRESSEL¹, MICHAEL MUTHIG¹, and THEYENCHERI NARAYANAN² — ¹Stranski Laboratorium, Institut für Chemie, Technische Universität Berlin, Berlin, Germany — ²European Synchrotron Radiation Facility (ESRF), Grenoble, France

In our experiments fast formation kinetics was studied by coupling the stopped-flow technique to high-flux SANS/SAXS instruments, allowing to obtain detailed structural information with a time-resolution of 5-50 ms. For the case of forming monodisperse unilamellar vesicles takes place in a way purely governed by diffusion and proceeds via a disk-like intermediate state. Further aging processes can be observed which are related to the stability of the vesicles. The structural progression of such systems can be modelled by simulations which allow to understand the aging processes in terms simple coalescence processes. Based on the detailed knowledge of the formation process it was then possible to manipulate it by the admixture of amphiphilic copolymers. By doing so systematic control over the vesicle size can be exercised and in addition the presence of the copolymer enhances the vesicle stability largely.

In summary, based on knowing the pathway of the formation of the unilamellar vesicles it can be controlled by the presence of the copolymers and thereby shaping of vesicles occurs in a systematic fashion.