

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

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Overview of Invited Talks and Sessions

(Lecture rooms: ZEU 114, 222, 260; Posters: P1, P2, P3)

Invited Talks

CPP 1.1	Mon	13:15–13:45	HSZ 02	Semicrystalline polymers - pathway of crystallization and deformation properties — ●GERT STROBL
CPP 2.1	Mon	9:30–10:00	ZEU 222	Structure-property relations in perylene bisimids: Charge mobility, exciton diffusion and singlet exciton fission — ●FERDINAND GROZEMA
CPP 3.5	Mon	10:30–11:00	ZEU 260	Role of heterogeneous structures and dynamics for transport properties of complex fluids: Insights from molecular dynamics simulations — ●MICHAEL VOGEL
CPP 8.4	Mon	15:45–16:15	ZEU 222	Controlled crystallization of semiconducting polymer thin films — ●SABINE LUDWIGS
CPP 9.1	Mon	15:00–15:30	ZEU 260	Self-assembly of soft colloids into meso-, para-, and quasicrystals — ●STEPHAN FOERSTER, ALEXANDER EXNER, SABINE ROSENFELDT, PETER LINDNER, JAN PERLICH
CPP 17.1	Tue	9:30–10:00	ZEU 260	Glassy dynamics of polymers in geometrical confinement: From nanometric layers to condensed isolated chains — ●FRIEDRICH KREMER
CPP 17.6	Tue	11:15–11:45	ZEU 260	Molecular Dynamics simulations of the glass transition in 1,4-polybutadiene confined by graphite walls — ●WOLFGANG PAUL, MATHIEU SOLAR, KURT BINDER
CPP 24.3	Tue	15:30–16:00	ZEU 260	Ion Conducting Polymers for Fuel Cells and Batteries: Where Polymer-chemistry meets Electrochemistry — ●KLAUS-DIETER KREUER
CPP 25.1	Tue	15:00–15:30	ZEU 222	Superhydrophobic Arrays of Functional Janus Micropillars — ●DORIS VOLLMER, PERIKLIS PAPAPOPOULOS, LENA MAMMEN, CLEMENS WEISS, HANS-JUERGEN BUTT
CPP 28.1	Wed	9:30–10:00	ZEU 222	Rheo-imaging of Polymer Networks — ●NORBERT WILLENBACHER
CPP 35.1	Wed	15:00–15:30	ZEU 222	Fabrication of 3D Cell Structures Using Self-Folding Polymer Films — ●LEONID IONOV
CPP 35.10	Wed	17:45–18:15	ZEU 222	Biopolymer Network Mechanics: Nonlinearity and Hierarchy. — ●CORNELIS STORM
CPP 39.1	Thu	9:30–10:00	ZEU 260	Clustering and phase separation of repulsive self-propelled discs — ●THOMAS SPECK
CPP 41.13	Thu	12:45–13:15	ZEU 222	Growth kinetics of metal nanoparticles on polymer surfaces — ●EZZELDIN METWALLI
CPP 42.5	Thu	10:30–11:00	ZEU 114	Tribology of colloidal systems — ●CLEMENS BECHINGER
CPP 42.6	Thu	11:00–11:30	ZEU 114	Contact and Friction of Rough Adhesive Surfaces — ●MARK ROBINS, LARS PASTEWKA, TRISTAN SHARP
CPP 43.1	Thu	11:45–12:15	ZEU 114	Dynamics and thermodynamics of glassy polymers below the glass transition temperature — ●DANIELE CANGIALOSI
CPP 48.5	Thu	16:00–16:30	ZEU 250	Universal aspects of chromosome folding — ●ANGELO ROSA
CPP 50.1	Thu	15:00–15:30	ZEU 114	Microscopic investigation of creep in glasses — TATJANA SENTJABRSKAJA, PINAKI CHAUDHURI, WILSON POON, JÜRGEN HORBACH, STEFAN EGELHAAF, ●MARCO LAURATI

CPP 50.2	Thu	15:30–16:00	ZEU 114	Getting into shape: Jamming of frictional particles. — •MATTHIAS SCHRÖTER, JEAN-FRANÇOIS MÉTAYER, FRANK RIETZ, MAX NEUDECKER
CPP 52.7	Thu	16:45–17:15	ZEU 222	Threading DNA through nanopores for biosensing applications — •MARIA FYTA
CPP 57.1	Fri	10:45–11:15	ZEU 260	Crystallization in Food — •HANS JÖRG LIMBACH, KONSTANTIN KOSCHKE, DAVIDE DONADIO
CPP 57.4	Fri	11:45–12:15	ZEU 260	Soft Matter Multi-Scale Food Physics - Texture, Taste and Aroma — •THOMAS VILGIS
CPP 58.1	Fri	9:30–10:00	ZEU 114	Probe Rheology with Neutron Scattering — •WIM PYCKHOUT-HINTZEN

Invited talks of the joint symposium SYMO

See SYMO for the full program of the symposium.

SYMO 1.1	Mon	9:30–10:00	HSZ 02	Molecular quantum spintronics with single-molecule magnets — •WOLFGANG WERNSDORFER
SYMO 1.2	Mon	10:00–10:30	HSZ 02	EPR Studies of Rare-Earth Molecular Nanomagnets — •STEPHEN HILL, SANHITA GHOSH, DORSA KOMIJANI, SALVADOR CARDONA-SERRA, JOSE-JAIME BALDOVI, YAN DUAN, ALEJANDRO GAITA-ARINO, EUGENIO CORONADO
SYMO 1.3	Mon	10:45–11:15	HSZ 02	On-surface magnetochemistry of spin-bearing metalorganic molecules — •PETER M. OPPENEER, KARTICK TARAFDER, EHESAN ALI, NIRMALYA BALLAV, CHRISTIAN WÄCKERLIN, THOMAS A. JUNG
SYMO 1.4	Mon	11:15–11:45	HSZ 02	Interfacing single-molecule magnets with metals — •ANDREA CORNIA, VALERIA LANZILOTTO, LUIGI MALAVOLTI, MATTEO MANNINI, MAURO PERFETTI, LUCA RIGAMONTI, ROBERTA SESSOLI
SYMO 1.5	Mon	11:45–12:15	HSZ 02	Linking magnetic molecules to themselves, to others and to surfaces — •RICHARD WINPENNY

Invited talks of the joint symposium SYMS

See SYMS for the full program of the symposium.

SYMS 1.1	Wed	9:30–10:00	HSZ 02	Imaging and manipulation of single functional molecules on surfaces — •LEONHARD GRILL
SYMS 1.2	Wed	10:00–10:30	HSZ 02	Adiabatic quantum motors — •FELIX VON OPPEN
SYMS 1.3	Wed	10:30–11:00	HSZ 02	Operation of molecular devices and machines on surfaces — •SAW WAI HLA
SYMS 1.4	Wed	11:15–11:45	HSZ 02	Driving and Controlling Molecular Surface Rotors with a Terahertz Electric Field — •RAYMOND DEAN ASTUMIAN
SYMS 1.5	Wed	11:45–12:15	HSZ 02	Unidirectional motion by inelastic electron tunneling — •KARL-HEINZ ERNST

Invited talks of the joint symposium SYCP

See SYCP for the full program of the symposium.

SYCP 1.1	Thu	9:30–10:00	HSZ 02	Why do polymer collapse and polymer topology frustrate each other — •ALEXANDER Y. GROSBURG
SYCP 1.2	Thu	10:00–10:30	HSZ 02	Nanoscopy of nuclear Genome Structure — •CHRISTOPH CREMER
SYCP 1.3	Thu	10:30–11:00	HSZ 02	Blood Clotting Inspired Polymer Physics — •ALFREDO ALEXANDER-KATZ
SYCP 1.4	Thu	11:15–11:45	HSZ 02	Modeling dynamic spatial genome organization in yeast — •CHRISTOPHE ZIMMER
SYCP 1.5	Thu	11:45–12:15	HSZ 02	Ring polymers in the melt state: the physics of crumpling — •RALF EVERAERS, ANGELO ROSA

Sessions

CPP 1.1–1.1	Mon	13:15–13:45	HSZ 02	Semocrystalline Polymers (joint session with HL)
CPP 2.1–2.9	Mon	9:30–12:15	ZEU 222	Organic Electronics and Photovoltaics (joint session with DS/HL/O) I
CPP 3.1–3.9	Mon	9:30–12:15	ZEU 260	Ionic Liquids
CPP 4.1–4.11	Mon	9:30–12:30	ZEU 114	Crystallization, Nucleation and Self Assembly I
CPP 5.1–5.7	Mon	10:45–12:30	POT 081	Energy Materials: Water Splitting, Batteries, and Supercapacitors (original: HL, joined by CPP)
CPP 6.1–6.8	Mon	10:30–13:15	TRE Ma	Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale (original: O, joined by CPP)
CPP 7.1–7.1	Mon	9:30–10:15	GER 37	Invited Talk by Martin Fally: Optics with Neutrons using Holographic Gratings (original: DF, joined by CPP, TT, KR)
CPP 8.1–8.10	Mon	15:00–18:00	ZEU 222	Organic Electronics and Photovoltaics (joint session with DS/HL/O) II
CPP 9.1–9.10	Mon	15:00–18:00	ZEU 260	Crystallization, Nucleation and Self Assembly II
CPP 10.1–10.5	Mon	15:00–16:15	ZEU 114	Wetting, Micro and Nanofluidics
CPP 11.1–11.8	Mon	16:30–18:30	ZEU 114	Interfaces and Thin Films I
CPP 12.1–12.7	Mon	15:00–17:45	HÜL 186	Focus Session: Feedback Control of Nonlinear Soft and Hard Matter Systems (original: DY, joined by CPP)
CPP 13.1–13.9	Mon	15:00–17:30	ZEU 146	Glasses (original: DY, joined by DF, CPP)
CPP 14.1–14.10	Mon	16:00–18:45	TRE Ma	Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale II (original: O, joined by CPP)
CPP 15.1–15.7	Mon	18:00–19:45	CHE 91	Organic Electronics and Photovoltaics A (original: DS, joined by CPP, HL, O)
CPP 16.1–16.13	Tue	9:30–13:00	ZEU 114	Interfaces and Thin Films II
CPP 17.1–17.10	Tue	9:30–12:45	ZEU 260	Transport and Confinement I
CPP 18.1–18.12	Tue	9:30–12:45	ZEU 222	Wetting, Superamphiphobicity, Micro- and Nanofluidics I
CPP 19.1–19.60	Tue	9:30–13:00	P1	Poster Session 1 (joint session with BP)
CPP 20.1–20.7	Tue	9:30–11:30	ZEU 118	Complex Fluids and Soft Matter (original: DY, joined by CPP, BP)
CPP 21.1–21.9	Tue	10:00–12:30	POT 081	Organic Semiconductors: Photovoltaics (original: HL, joined by CPP, DS)
CPP 22.1–22.9	Tue	10:30–13:15	TRE Ma	Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale III (original: O, joined by CPP)
CPP 23.1–23.4	Tue	15:00–16:00	ZEU 114	Interfaces and Thin Films III
CPP 24.1–24.3	Tue	15:00–16:00	ZEU 260	Transport and Confinement II
CPP 25.1–25.3	Tue	15:00–16:00	ZEU 222	Wetting, Superamphiphobicity, Micro- and Nanofluidics II
CPP 26.1–26.7	Tue	14:00–15:45	POT 081	Organic Semiconductors: Transistors and OLEDs (original: HL, joined by CPP, DS)
CPP 27.1–27.12	Wed	9:30–12:45	ZEU 260	Organic Electronics and Photovoltaics (joint session with DS/HL/O) III
CPP 28.1–28.10	Wed	9:30–12:30	ZEU 222	(Hydro) Gels and Elastomers
CPP 29.1–29.12	Wed	9:30–12:45	ZEU 114	Colloids and Complex Liquids I
CPP 30.1–30.5	Wed	9:30–12:15	HSZ 02	Molecular Switches and Motors at Surfaces (original: SYMS, joined by CPP, O)
CPP 31.1–31.10	Wed	10:30–13:15	TRE Ma	Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale IV (original: O, joined by CPP)
CPP 32.1–32.3	Wed	11:45–12:45	WIL B321	Glasses (original: DF, joined by CPP, DY)
CPP 33.1–33.12	Wed	9:30–13:00	HÜL 386	Cytoskeleton (original: BP, joined by CPP)
CPP 34.1–34.12	Wed	15:00–18:15	ZEU 260	Organic Electronics and Photovoltaics (joint session with DS/HL/O) IV
CPP 35.1–35.10	Wed	15:00–18:15	ZEU 222	Biomaterials and Biopolymers (joint session with BP) I
CPP 36.1–36.12	Wed	15:00–18:15	ZEU 114	Colloids and Complex Liquids II
CPP 37.1–37.73	Wed	15:00–19:00	P3	Poster Session 2

CPP 38.1–38.11	Wed	16:00–19:15	TRE Ma	Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale V (original: O, joined by CPP)
CPP 39.1–39.5	Thu	9:30–11:00	ZEU 260	Active Colloids
CPP 40.1–40.6	Thu	11:15–12:45	ZEU 260	Colloids and Complex Liquids III
CPP 41.1–41.13	Thu	9:30–13:15	ZEU 222	Nanoparticles and Composite Materials
CPP 42.1–42.6	Thu	9:30–11:30	ZEU 114	Friction and Lubrication
CPP 43.1–43.3	Thu	11:45–12:45	ZEU 114	Glasses and Glass Transition (joint session with DY/DF) I
CPP 44.1–44.11	Thu	9:30–12:30	ZEU 118	Charged Soft Matter I
CPP 45.1–45.5	Thu	9:30–12:15	HSZ 02	The Collapsed State of Polymers: From Physical Concepts to Applications and Biological Systems (symposium, CPP/DY/BP)
CPP 46.1–46.9	Thu	9:30–12:30	HÜL 186	Focus Session: Slow Dynamics in Glasses and Granular Matter I (original: DY, joined by CPP)
CPP 47.1–47.10	Thu	10:30–13:15	TRE Ma	Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale VI (original: O, joined by CPP)
CPP 48.1–48.8	Thu	15:00–17:30	ZEU 250	The Collapsed State of Polymers: From Physical Concepts to Applications and Biological Systems (joint session with BP)
CPP 49.1–49.5	Thu	17:00–18:15	ZEU 260	Polymer Dynamics I
CPP 50.1–50.7	Thu	15:00–17:30	ZEU 114	Glasses and Glass Transition (joint session with DY/DF) II
CPP 51.1–51.8	Thu	15:00–17:00	ZEU 118	Charged Soft Matter II
CPP 52.1–52.13	Thu	15:00–18:45	ZEU 222	Biomaterials and Biopolymers (joint session with BP) II
CPP 53.1–53.8	Thu	17:45–19:45	CHE 91	Organic Electronics and Photovoltaics B (original: DS, joined by CPP, HL, O)
CPP 54.1–54.85	Thu	15:00–19:00	P2	Poster Session 3
CPP 55	Thu	19:00–20:00	ZEU 222	Mitgliederversammlung des Fachverbandes CPP
CPP 56.1–56.4	Fri	9:30–10:30	ZEU 260	Colloids and Complex Liquids IV
CPP 57.1–57.4	Fri	10:45–12:15	ZEU 260	Physics of Food
CPP 58.1–58.6	Fri	9:30–11:15	ZEU 114	Polymer Dynamics II
CPP 59.1–59.8	Fri	9:30–12:15	HÜL 186	Focus Session: Slow Dynamics in Glasses and Granular Matter II (original: DY, joined by CPP, DF)
CPP 60.1–60.9	Fri	10:15–12:30	POT 051	Organic Semiconductors: Material Properties (original: HL, joined by CPP,DS)

Mitgliederversammlung des Fachverbandes Chemische Physik und Polymerphysik - Annual General Meeting of the Chemical and Polymer Physics Division

Donnerstag, 03.04.2014 19:00–20:00 ZEU222

- Bericht des Sprechers
- Wahl des Sprechers 2016/2017
- Verschiedenes

CPP 1: Semicrystalline Polymers (joint session with HL)

Lecture on the occasion of the Robert-Wichard-Pohl-Preis 2014 awarded to Gert Strobl

Time: Monday 13:15–13:45

Location: HSZ 02

Invited Talk CPP 1.1 Mon 13:15 HSZ 02
Semicrystalline polymers - pathway of crystallization and deformation properties — ●GERT STROBL — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, 79104 Freiburg

On cooling a polymer melt, plate-like crystals with thicknesses in the nano-range are nucleated and grow in the two lateral directions. The final structure is semicrystalline and composed of stacks of such crystallites separated by entangled fluid chain sequences. Structure parameters vary with the crystallization temperature which can be chosen far below the equilibrium melting point, down to the transition into

the glassy state. The question about the mechanism of polymer crystallization has always been a central issue in polymer physics. Time- and temperature dependent X-ray scattering experiments carried out during the last two decades now led to the establishment of a set of laws which control the structure formation out of the entangled melt, recrystallization processes, and the final melting. The laws indicate the participation of an intermediate mesomorphic phase in the crystal formation process. The peculiar deformation behaviour of polymeric materials reflects their semicrystalline structure, including in a coupled fashion both the rubber-like properties of the fluid parts and the elasto-plastic properties of the crystallites.

CPP 2: Organic Electronics and Photovoltaics (joint session with DS/HL/O) I

small molecules, hybrid materials

Time: Monday 9:30–12:15

Location: ZEU 222

Invited Talk CPP 2.1 Mon 9:30 ZEU 222
Structure-property relations in perylene bisimides: Charge mobility, exciton diffusion and singlet exciton fission — ●FERDINAND GROZEMA — Delft University of Technology, Department of Chemical Engineering, Delft, The Netherlands

Perylene diimides (PDIs) represent a class of materials that is promising for application as the active layer in field effect transistors and as an electron accepting material in organic photovoltaic cells. The electronic properties of PDI-based materials strongly depend on the supramolecular order in the material. Therefore, a thorough understanding of the relation between the electronic properties and the organization on the molecular scale can result in design rules for the synthesis of new π -conjugated organic molecules.

To achieve this we have performed a combined experimental and theoretical study of the electronic properties of a large library of PDI derivatives that differ in the side chains, resulting in subtle differences in the crystal structure. By time-resolved microwave conductivity measurements we show a strong correlation between the supramolecular organization and the charge carrier mobility, with a maximum mobility of 0.41 cm²/Vs. Singlet exciton fission, a process in which a singlet excited state is efficiently converted into two triplets, is also found to be strongly dependent on the supramolecular organization.

This comprehensive study shows that the engineering of the supramolecular organization in PDIs and conjugated molecules in general is a viable approach to tailor a variety of electronic properties of such materials over a wide range.

CPP 2.2 Mon 10:00 ZEU 222

Influence of morphology on organic solar cell performance comparing crystalline diindenoperylene (DIP) and its amorphous derivative tetraphenylidibenzoperiflanthene (DBP) — ●STEFAN GROB, MARK GRUBER, ULRICH HÖRMANN, THERESA LINDERL, and WOLFGANG BRÜTTING — 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, these 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 and thus a smaller short-circuit current density. The difference in morphology also leads to different coupling between donor and acceptor molecules at the interface. As a consequence there is an appreciable distinction in the recombination processes occurring within the solar cell. We investigate this phenomenon by temperature-dependent j-V-measurements, electro-

luminescence and photothermal deflection spectroscopy. Based on these results, we discuss the influence of different film structure and morphology on electrical transport and device performance.

CPP 2.3 Mon 10:15 ZEU 222

Spray deposition of zinc oxide nanostructured films for applications in dye-sensitized solar cells — ●KUHUSARKAR¹, ERIK V. BRADEN¹, STEFAN POGORZALEK¹, SHUN YU², STEPHAN V. ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching — ²DESY, Notkestr. 85, 22607 Hamburg

Zinc oxide (ZnO) has emerged as a suitable alternative to titania (TiO₂) in the recent years in the field of dye-sensitized solar cells (DSSCs). The inorganic metal oxide films for DSSCs are highly desirable to have an increased surface for enhanced adsorption of a photosensitizer. Hence, nanostructured films of ZnO are synthesized from a solution based approach. Different deposition techniques are investigated to have a significant film thickness for a considerable amount of light absorption. In this respect, spray deposition is shown to be a highly efficient and scalable technique to produce films matching the above-mentioned criteria. Surface as well as bulk morphology of the films have been studied using SEM and GISAXS. These ZnO films are successfully shown to provide good performance in a dye-sensitized solar cell with the highest short circuit current density reported so far.

CPP 2.4 Mon 10:30 ZEU 222

Extremely Thin Absorber Solar Cells based on Sb₂S₃ — ●EUGEN ZIMMERMANN, JONAS WEICKERT, THOMAS PEADLER, JAMES DORMAN, and LUKAS SCHMIDT-MENDE — Universität Konstanz

The introduction of nanostructured metal oxides as electron acceptor resulted in the concept of extremely thin absorber solar cells. Thus, low cost fabricated inorganic semiconductors like Sb₂S₃ can be utilized as sensitizer, which typically possess promising properties, such as a tunable band gap and high extinction coefficient. However, optimization of the fabrication process and a detailed characterization of intrinsic properties is unavoidable in order to find the best device architecture and suitable material combinations for highly efficient solar cells. For this purpose, chemical bath deposition conditions and parameters have been examined and resulted in a detailed recipe for fabrication of high quality Sb₂S₃ coatings. In combination with optimized layer thicknesses of P3HT, efficiencies of up to 3.2% could be achieved in flat heterojunction architecture. In order to identify intrinsic limitations, comparative measurements with P3HT:PCBM cells have been, revealing monomolecular recombination processes of excitons, a potential dependency of charge separation, and long charge carrier pathways as main loss mechanisms of fabricated flat heterojunction cells. In addition, investigation of several hole transport materials (HTM) revealed a disadvantageous influence on charge generation due to the parasitic absorption of light by the HTM. Based on these results, the use of nanostructured metal oxides in combination with transparent HTMs is proposed to possibly overcome some of the found limitations.

CPP 2.5 Mon 10:45 ZEU 222

Towards low-temperature synthesis of polymer/titania hybrid films for application in photovoltaics — MARTIN A. NIEDERMEIER¹, MONIKA RAWOLLE¹, ERIK V. BRADEN¹, KUHU SARKAR¹, EVA M. HERZIG², VOLKER KÖRSTGENS¹, and ●PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — ²TU München, Munich School of Engineering, James-Franck-Str. 1, 85748 Garching

In a hybrid solar cell an inorganic matrix, such as titania, is combined with a hole-conducting polymer to form a so-called bulk heterojunction. The functionality of such a system depends strongly on the quality of the polymer/semiconductor interface. A very common approach to fabricate that interface is the so-called backfilling of the existing inorganic matrix with the conducting polymer. This approach is generally a two-step process, as the fabrication of the inorganic matrix usually involves high temperatures, which destroy all organic material present in the system. To date the subsequent backfilling of that matrix remains challenging, since a lot of problems have to be overcome. A workaround to these problems is promised by a low-temperature sol-gel process, in which the polymer and the inorganic semiconductor network are fabricated simultaneously. Approaches towards such low-temperature synthesis of polymer/titania hybrid films for application in photovoltaics are presented. These novel routes make use of special tailored block copolymers as structure directing agent. Film morphology and device function are investigated.

15 min break

CPP 2.6 Mon 11:15 ZEU 222

Photoinduced charge transfer in CuInS₂ nanocrystal/polymer composites — ●RANY MIRANTI¹, YULIAR FIRDAUS², CHRISTOPHER KRAUSE¹, MARK VAN DER AUWERAER², HOLGER BORCHERT¹, and JÜRGEN PARISI¹ — ¹Univ. of Oldenburg, Dept. of Physics, Energy and Semiconductor Research Laboratory, 26129 Oldenburg, Germany — ²Lab. for Photochemistry & Spectroscopy, Div. of Mol. Imaging & Photonics, Chemistry Dept., Katholieke Universiteit Leuven, Celestijnenlaan 200 F B-3001 Heverlee, Belgium.

The photoinduced excited states and the effects properties of charge transfer in CuInS₂ (CIS) nanocrystal/polymer composites were studied by applying quasi steady-state photoinduced absorption (PIA) and steady state photoluminescence as well as time-resolved photoluminescence. The time-resolved properties and excited state dynamics of our systems were studied using the time-correlated single photon counting (TCSPC) technique. We used two different systems of composites with two different kind of polymer, i.e. poly(3-hexylthiophene) (P3HT) and poly[2,6-(4,4-bis-(2-ethylhexyl)-4H-cyclopenta[2,1-b;3,4-b']dithiophene)-alt-4,7-(2,1,3-benzothiadiazole)] (PCPDTBT). Optical absorption and emission spectra of thin films of CIS nanocrystal/polymer composites exhibit several interesting features such as luminescence quenching and polaronic photoinduced absorption (PIA) indicating photoinduced charge transfer. The effect of different organic ligands surrounding the CIS nanocrystals on the charge separation process in CIS nanocrystal/polymer composites will be presented as well.

CPP 2.7 Mon 11:30 ZEU 222

Structured growth of ZnO for light trapping enhancement in organic solar cells — ●NIVEDITA YUMNAM and VEIT WAGNER — Jacobs University, 28759 Bremen, Germany

Organic photovoltaic cells are promising candidates for large-area and low-cost production of solar cells. However, their performance is limited due to the short diffusion length of excitons and low absorption in the active semiconductor layer. The absorption of light can be en-

hanced by incorporating ZnO nanostructures, which act as scattering centres and hence, they increase the optical path length of light. Our work focuses on the investigation of light trapping mechanism of solar cells based on electrochemically grown ZnO nanorod and active layer of conjugated polymer P3HT and PCBM. The size and the structure of the ZnO nanorods are varied by changing the parameters of electrochemical deposition. Angle resolved scattering measurements are employed to investigate the amount of light scattered by the nanorods. These results are correlated to the performance of the solar cell determined from electrical measurements.

CPP 2.8 Mon 11:45 ZEU 222

Temperature-dependent molecular orientation of the organic semiconductor PTCDI-C₈: Optical and structural properties — ●SEBASTIAN BOMMEL^{1,2}, LINUS PITHAN², CHRISTOPHER WEBER², ANTON ZYKOV², GONZALO SANTORO¹, STEPHAN V. ROTH¹, JÖRG MEGOW², and STEFAN KOWARIK² — ¹Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, D-22607 Hamburg, Germany — ²Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489 Berlin, Germany

Optical and structural properties of molecular materials are not only essential for the rational design of opto-electrical devices, but also for the understanding of intermolecular interactions. Here, we report on the structural and optical properties of the organic semiconductor PTCDI-C₈ investigated by temperature-dependent Grazing Incidence X-ray Diffraction (GIXD) and photoluminescence (PL) measurements. Our *in situ* studies yield a large impact of temperature on unit cell parameters and optical transitions. The energy of the optical transition E₁₀-E₀₁ in the PL spectra shifts from 1.80 eV for 273 K to 1.85 eV for 413 K. Furthermore, a rearrangement of the molecular ensemble was found, indicated by a large change of the beta-angle of the PTCDI-C₈ unit cell from 107° (273 K) to 102° (413 K). The influence of these structural changes, which are an indication for a change of molecular orientation with temperature, on the optical properties will be discussed in detail. Additionally, the structural and optical properties are supported by temperature-dependent molecular dynamics (MD) simulation based calculations.

CPP 2.9 Mon 12:00 ZEU 222

Highly Efficient Silicon/Polythiophene Hybrid Solar Cell Devices — ●MATTHIAS ZELMEIER¹, JOHANNES FRISCH², SILVIA JANIEZ³, NORBERT KOCH², JÖRG RAPPICH¹, and NORBERT NICKEL¹ — ¹Helmholtz-Zentrum Berlin, Institut für Silizium Photovoltaik, Kekuléstr. 5, D-12489 Berlin — ²Humboldt-Universität zu Berlin, Institut für Physik, Brook-Taylor-Str. 6, D-12489 Berlin — ³Fraunhofer-Institut für Angewandte Polymerforschung IAP, Abteilung Polymere und Elektronik, Geiselbergstr. 9, D-14476 Potsdam

Highly efficient hybrid solar cell devices based on crystalline silicon with three different solution processed polymer emitter layers are realized. The inorganic part of the device is optimized with a hole-selective back contact (BSF) and a low defect density hot water oxide ($D_{it}=2 \times 10^{-12} \text{ eV}^{-1} \text{ cm}^{-2}$), which provides the necessary wetting properties for the solution processed emitter layers. The applied polymer materials, e.g. poly(3-hexylthiophene-2,5-diyl) (P3HT), poly(3-[3,6-dioxaheptyl]-thiophene) (P3DOT), and poly(3-[2,5,8-trioxanonyl]-thiophene) (P3TOT), differ mainly in the oxygen content in the side groups. Substituting the alkyl chains attached to the thiophene rings with ether groups leads to a modified layer formation during spin coating. The results of the optical, electrical and structural characterization of the polymer layers is correlated to the key figures in the final devices. The open circuit voltage V_{OC} increases from 0.3 V to 0.5 V and the short circuit current j_{SC} increases from 15.2 mA cm⁻² up to 28.3 mA cm⁻² in the sequence P3HT, P3DOT, P3TOT and results in a power conversion efficiency close to 10 % for a planar Si/P3TOT device.

CPP 3: Ionic Liquids

Time: Monday 9:30–12:15

Location: ZEU 260

CPP 3.1 Mon 9:30 ZEU 260

A joint theoretical/experimental study of the influence of different FSI:TFSI ratios on lithium dynamics in ionic liquids — ●VOLKER LESCH, SEBASTIAN JEREMIAS, ARIANNA MORETTI, STEFANO PASSERINI, and ANDREAS HEUER — Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster

Because of their properties ionic liquids are promising materials for different applications like catalysis or electrochemical applications. The broad range of possible ionic liquids makes it possible to adjust the ionic liquids to special requirements but it is also a big challenge due to synthesis and characterization. MD-simulations are a powerful tool to get detailed information about the microscopic properties of ionic liquid. However, suitable simulations require polarisable force fields. In this study we use the polarisable force field APPLE&P from Wasatch Molecular Inc. Our main goal was to investigate the influence of different FSI:TFSI (bis(fluorosulfonyl)imide:bis(trifluorosulfonyl)imide) ratios on the lithium ion transport. Note that both anions have complementary properties to improve electrolytes like the electrochemical stability window or film forming abilities. A very good agreement between experimental and theoretical results enable a microscopic investigation of transport properties and complex formation via MD simulations. We determine residence times of FSI and TFSI inside the first coordination shell of lithium ions and also in a lithium lithium complex. In these complexes TFSI acts as a bridge and connects both lithium ions. We analyzed these complexes with respect to the residence times of anions and the life time of the complete complex.

CPP 3.2 Mon 9:45 ZEU 260

The influence of different ion-species on ionic conductivity in polymer electrolytes mixed with ionic liquids — ●JOYJIT CHATTORAJ and ANDREAS HEUER — Institut für Physikalische Chemie, Westfälische Wilhelm Universität Muenster, Corrensstr. 28/30, 48149 Münster, Germany

We perform molecular dynamics (MD) simulations on a system of poly(ethylene oxides) PEO chains mixed with Li-cations and TFSI-anions and additionally the MPPY-TFSI ionic liquid over a broad range of temperatures and varying ionic liquid concentrations. This is a prototype of the solid polymer electrolyte which promises an improved ionic conductivity for Li-metal batteries at room temperature. Here we investigate the influence of different ion-species associations on ionic conductivity. In general for MD simulations ionic conductivity is estimated from the mean square displacement MSD of ions using the Nernst-Einstein equation. The collective MSD is expressed as a sum of self and cross terms. We show that the cross terms have peculiar characteristics due to the conservation of momentum. To be specific we find that the cross MSD of similar ions lowers the collective MSD and the cross MSD of different type of ions enhances the MSD and so ionic conductivity. The peculiarity in the cross MSD values is then investigated via looking upon the directional and mobility correlations of ions over space and time. A phenomenological model is proposed to further explain the influence of ion associations on the ionic conductivity and the results are compared with experiments.

CPP 3.3 Mon 10:00 ZEU 260

Effect of ionic liquid on the surface energy of carbon black and reinforcement of high performance elastomers — ●FRANK FLECK, PATRICK STRATMANN, and MANFRED KLÜPPEL — Deutsches Institut für Kautschuktechnologie e.V., Eupener Straße 33, 30519 Hannover

In the present work the polymer-filler interaction of reinforced elastomers is investigated with different experimental methods. To understand how the surface influences the properties of the system, carbon black was modified with the ionic liquid 1-allyl-3-methylimidazolium chloride (AMIC).

To quantitatively describe the modification of the surface activity, the surface of the filler was characterized by static gas adsorption measurements. To get information about the interaction strength of the monomers of typical diene rubbers, 1-butene was used as adsorbate. With that the energy distribution function is calculated from the adsorption isotherms. It is found that the ionic liquid molecules tend to interact with the high energetic sites of the carbon black and therefore the adsorption strength of polymer chains at the filler surface

is reduced in the case of nonpolar rubbers. By using more polar elastomers the cations of the ionic liquid can interact with the polar groups of the polymer chain, which influences the polymer-filler interaction in a different way than for nonpolar systems.

Based on flocculation experiments it can be shown, that the mechanism of forming a filler network is strongly influenced by the modification with ionic liquids.

CPP 3.4 Mon 10:15 ZEU 260

Volatility of ionic liquids at the nanoscale by means of ultrafast scanning calorimetry — ●MATHIAS AHRENBERG¹, MARCEL BRINCKMANN¹, JÜRN W.P. SCHMELZER¹, MARTIN BECK², CHRISTIN SCHMIDT³, OLAF KESSLER², UDO KRAGL³, SERGEY P. VEREVKIN³, and CHRISTOPH SCHICK¹ — ¹Institute of Physics, University of Rostock, Wismarsche Str. 43-45, 18051 Rostock, Germany — ²Faculty of Mechanical Engineering and Marine Technology, University of Rostock, Albert-Einstein-Str. 2, 18059 Rostock, Germany — ³Institute of Chemistry, University of Rostock, Albert-Einstein-Str. 3a, 18059 Rostock, Germany

The determination of vaporization enthalpies of extremely low volatile ionic liquids is challenging and time consuming due to the low values of vapor pressure. In addition, these liquids tend to decompose already at temperatures where the vapor pressure is still low. Conventional methods for determination of vaporization enthalpies are thus limited to temperatures below the decomposition temperature. Here we present a new method for the determination of vaporization enthalpies of such liquids using differential fast scanning calorimetry. We have developed and proven this method using [EMIm][NTf₂] at temperatures up to 750 K and in different atmospheres. It was demonstrated that evaporation is still the dominating process of mass loss even at such highly elevated temperatures. Since the method allows very high heating rates (up to 100000 K/s), much higher temperatures can be reached in the measurement of the mass loss rate as compared to common devices without significant decomposition of the ionic liquid.

Invited Talk

CPP 3.5 Mon 10:30 ZEU 260

Role of heterogeneous structures and dynamics for transport properties of complex fluids: Insights from molecular dynamics simulations — ●MICHAEL VOGEL — Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstr. 6, 64289 Darmstadt, Germany

A large variety of complex fluids show heterogeneous structures and dynamics, e.g., ionic liquids can exhibit concentration fluctuations, which manifest themselves in mobility variations. In the vicinity of solid interfaces, inhomogeneities of structures and dynamics are often particularly pronounced. Any heterogeneities on nanoscopic scales can have severe consequences for material behaviors and functions on macroscopic scales. Molecular dynamics simulations are a powerful tool to determine molecular structure and dynamics on different scales. We exploit this capability to develop a fundamental understanding of macroscopic mass transport based on space-time characteristics of nanoscopic structural and dynamical heterogeneities. The studied examples include supercooled liquids, ionic liquids, and polymer melts. Moreover, we compare the liquid behavior in the bulk and at various interfaces, including biological surfaces.

15 min break

CPP 3.6 Mon 11:15 ZEU 260

Vibrational dynamics of the C-H stretch region of imidazolium based ionic liquids:[C₂mim][NTf₂] — ●TOBIAS ZENTEL¹, SUSANA CHATZIPAPADOPOULOS¹, MATTHIAS LÜTGENS¹, SERGEI D. IVANOV¹, STEFAN LOCHBRUNNER¹, RALF LUDWIG², and OLIVER KÜHN¹ — ¹Institut für Physik, Universität Rostock — ²Institut für Chemie, Universität Rostock

To understand the physico-chemical properties of ionic liquids, the knowledge of intermolecular interactions is of utmost importance. The ionic character of the molecules leads to strong Coulomb forces, but also a distinct hydrogen bond network exists [1]. In this contribution we focus on the dynamics of their hydrogen bonds under the influence of the fluctuating environment. Using force field based molecular dynamics (MD) simulation and ab initio methods as well as ultrafast

coherent anti Stokes Raman spectroscopy (CARS), the C-H stretch modes located on the imidazolium ring of the aprotic ionic liquid [C₂mim][NTf₂] are used as sensors for the hydrogen bond interactions.

Following Oxtoby et al. [2] the force projected on the C-H bonds is utilized to obtain frequency fluctuations and frequency correlation functions along the bulk MD trajectory. This allows to calculate dephasing times which in accord with CARS results show a distinct dependence on the H-bonding site. The force field results are scrutinized by DFT calculations.

[1] C. Roth et al. *New J. Phys.* **14**,105026 (2012)

[2] D. Oxtoby, D. Levesque, J. Weis *J.Chem.Phys* **68**,5528, 1978

CPP 3.7 Mon 11:30 ZEU 260

Electrospray ionization deposition of ultrathin ionic liquid films: [C₈C₁Im]Cl and [C₈C₁Im][Tf₂N] on Au(111) — ●FLORIAN RIETZLER, MARIUS PIERMAIER, ALEXEY DEYKO, HANS-PETER STEINRÜCK, and FLORIAN MAIER — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

We introduce a new method for preparing ultrathin ionic liquid (IL) films on surfaces by means of electrospray ionization deposition (ESID) under well defined ultra-high vacuum (UHV) conditions. In contrast to physical vapor deposition (PVD), ESID even allows the deposition of ILs, which are prone to thermal decomposition. We first investigated ultrathin [C₈C₁Im][Tf₂N] (=1-methyl-3-octyl-imidazolium bis(trifluoromethyl)imide) and [C₈C₁Im]Cl ESID-films on Au(111); [C₈C₁Im]Cl is an example of an IL that cannot be prepared as ultrathin film otherwise. [C₈C₁Im][Tf₂N] and [C₈C₁Im]Cl both form a wetting layer with a checkerboard arrangement with the cationic imidazolium ring and the anion adsorbed next to each other on the substrate and the alkyl chain pointing towards vacuum. Further deposition of [C₈C₁Im]Cl leads to a pronounced island growth on top of the wetting layer, which is independently confirmed by angle-resolved XPS and atomic force microscopy. This behavior contrasts the growth behavior found for [C₈C₁Im][Tf₂N], where layer-by-layer growth on top of the wetting layer is observed. The dramatic difference between both ILs is attributed to differences in the cation-anion interactions, and in the degree of order in the wetting layer of the two ILs.

CPP 3.8 Mon 11:45 ZEU 260

Orientation at Liquid Surfaces: XPS Studies on Functionalised and Reactive Ionic Liquids — ●INGA NIEDERMAIER¹, CLAUDIA KOLBECK¹, ALEXEY DEYKO¹, NICOLA TACCARDI², WEI WEI², PE-

TER WASSERSCHIED², HANS-PETER STEINRÜCK¹, and FLORIAN MAIER¹ — ¹FAU Erlangen, Phys. Chemie II — ²FAU Erlangen, Chem. Reaktionstechnik, Egerlandstr. 3, 91058 Erlangen

Ionic liquids (ILs) are molten salts with a melting point below 100 °C. Their extremely low vapour pressure allows using UHV-based surface science methods such as X-ray photoelectron spectroscopy (XPS). The liquid-vacuum interface of non-functionalised ILs with long alkyl chains has been studied thoroughly in the past.[1-2] At the surface, they generally exhibit a preferred orientation of their nonpolar alkyl moieties towards vacuum. Herein, we now present a detailed surface study of ILs carrying ether, thioether, amine and halogen functional groups. In addition, imidazolium based ILs methylated at the C(2) position are considered. From the angle-resolved XP spectra of all core levels, detailed information on surface enrichment of the functional groups and the arrangement of the ionic headgroups is derived. Furthermore, in-situ XPS of a reactive IL mixture[3] enables monitoring changes in surface segregation and orientation during course of the reaction.

Supported by the Cluster of Excellence - Engineering of Advanced Materials and DFG grant Ste 620/9-1.

[1] C. Kolbeck et al., *J. Phys. Chem. B*, **2009**, 113, 8682-8688.

[2] K. R. J. Lovelock et al., *J. Phys. Chem. B*, **2009**, 113, 2854-2864.

[3] C. Kolbeck et al., *Angew. Chem. Int. Edit.*, **2012**, 51, 2610-2613.

CPP 3.9 Mon 12:00 ZEU 260

Surface crystallization in the ionic liquid [C₂₂mim⁺][TFSI⁻] — ●JULIAN MARS¹, BINYANG HOU^{1,2}, PETER REICHERT^{1,3}, DIEGO PONTONI², HARALD REICHERT², OLEG KONOVOLAV², and MARKUS MEZGER^{1,3} — ¹Max-Planck-Institut für Polymerforschung, 55128 Mainz, Germany — ²European Synchrotron Radiation Facility, 38043 Grenoble, France — ³Johannes Gutenberg-Universität, 55128 Mainz, Germany

The near surface structure of 1-docosyl-3-methylimidazolium bis(trifluoromethane)sulfonimide ([C₂₂mim⁺][TFSI⁻]) was studied by x-ray reflectivity (XRR) and grazing incidence diffraction (GID). At high temperatures, an oscillating decaying electron density profile was observed by XRR experiments [1]. Up to 20°C above the bulk melting point, the formation of a discrete number of surface crystalline layers was detected by XRR. Their in-plane structure was studied by GID. Complementary bulk x-ray diffraction, differential scanning calorimetry, and petrographic microscopy measurements suggest that the observed surface structure is related to a metastable bulk phase.

[1] M. Mezger et al., *Proc. Natl. Acad. Sci. USA* **110**, 3733 (2013).

CPP 4: Crystallization, Nucleation and Self Assembly I

Time: Monday 9:30–12:30

Location: ZEU 114

CPP 4.1 Mon 9:30 ZEU 114

Self-assembly of quasicrystals in colloid-polymer mixtures — ●ERDAL C. OĞUZ, MATTHIAS SANDBRINK, and MICHAEL SCHMIEDEBERG — Heinrich-Heine-Universität Düsseldorf

By combining lattice sum calculations and Monte Carlo computer simulations, we investigate the stability of quasicrystals in colloid-polymer mixtures. In our model, the colloidal interactions are dictated by a repulsive Yukawa potential, whereas the presence of polymers yield an attractive depletion force between them. Hence, we obtain an isotropic pair interaction potential with multiple length scales that we use to support the two incommensurate length scales of the desired quasicrystalline structures. By minimizing the corresponding lattice sums, we determine the ground-state phase diagram (T=0) and we search for parameter sets where the system prefers quasicrystalline ordering rather than any other crystalline structure, i.e., we explain what polymer concentration, what depletion length, and what density are needed to grow quasicrystals with a given symmetry. For comparison and in order to extend the ground-state calculations to finite temperatures, we perform Monte Carlo computer simulations of our system. Therefore, our calculations and simulations explain how colloidal building blocks in experiments have to be designed in order to achieve the self-assembly of intrinsic colloidal quasicrystals.

CPP 4.2 Mon 9:45 ZEU 114

Testing nucleation theory for collidal crystals from estimates for the Laplace pressure in the fluid — ●ANTONIA STATT, PETER

VIRNAU, and KURT BINDER — Institut für Physik, JGU Mainz

We use a soft extension of the well-known effective Asakura Oosawa model [1] to study phase coexistence of a crystal "droplet" surrounded by liquid with Monte Carlo Simulations. In classical nucleation theory, the barrier of homogeneous nucleation is given by two contributions, the energy gain of creating a droplet and the energy loss due to surface tension of the new created interface. The enhancement of the pressure in the surrounding liquid in comparison to the coexistence pressure, the so-called Laplace pressure, can be measured via the virial theorem [2]. With this we are able to compare the predictions of the classical nucleation theory without suffering from ambiguities occurring when one needs a microscopic identification of the crystalline droplet.

[1] M. Dijkstra, R. van Roij and R. Evans, *Phys. Rev. E* **59**, 5744-5771, 1999

[2] D. Deb, A. Winkler, P. Virnau and K. Binder, *J. Chem. Phys.* **136**, 134710, 2012

CPP 4.3 Mon 10:00 ZEU 114

Guided assembly of nano-particles exploiting forces induced by 3D confinement — ●STEFAN FRINGES¹, COLIN RAWLINGS¹, HEIKO WOLF¹, URS DUERIG¹, MADHAVI KRISHNAN², and ARMIN KNOLL¹ — ¹IBM Research, 8803 Rüschlikon, Switzerland — ²Institute of Physical Chemistry, University of Zurich, 8057 Zurich, Switzerland

It has been shown previously that charged nanoparticles can be sta-

bilized in a static nano-fluidic slit due to the formation of the electric double layer. By shaping the topography of the confining interfaces, a trapping potential is established for the nanoparticle, which overcomes the Brownian motion and traps the nanosized object for several hours [1]. Here we demonstrate a mechanical setup capable of controlling the confining surfaces with sub-nanometer precision. By controlling the slit height, the strength of the trapping potential is directly controlled. The shape of the potential is also defined by the shape of the topography, which is carved out of a thermally decomposable polymer film by 3D thermal Scanning Probe Lithography (tSPL) [2]. The potential landscape is experimentally determined by observation of the particle motion at high frame rates using Interferometric scattering imaging. The undissociated polymer surface has a lower energy barrier for direct contact. We demonstrate that this energy barrier can be overcome at small separations, where the van der Waals force dominates providing stable deposition. In addition, the particles can be transferred to the substrate of choice by thermal decomposition of the polymer film.

[1] Krishnan et al., Nature 467, 692-695, 2010

[2] D. Pires, A.W. Knoll et al., Science 328(5979), 732-735, 2010

CPP 4.4 Mon 10:15 ZEU 114

Real-Time Observation of Non-Classical Protein Crystallization Kinetics — ●ANDREA SAUTER¹, GUDRUN LOTZE², FAJUN ZHANG¹, and FRANK SCHREIBER¹ — ¹Universität Tübingen, Institut für Angewandte Physik — ²European Synchrotron Radiation Facility, F-38043 Grenoble Cedex 9, France

We present a real-time study of protein crystallization for beta-lactoglobulin in the presence of CdCl₂ by small angle X-ray scattering (SAXS) and optical microscopy. In the presence of CdCl₂ both classical and non-classical crystallization can be found depending on the concentration of protein and salt. A phase diagram region can be identified in which real-time SAXS demonstrates the existence of an intermediate state prior to crystallization that cannot be explained by classical nucleation theory. It shows as a minimum at 0.48 nm⁻¹ and a maximum at 0.7 nm⁻¹ which become visible in the scattering curves after several minutes. With time, this new feature becomes more pronounced. In the next step, Bragg peaks appear and the position of the minimum shifts towards larger q values. The minimum regresses again and in the end, only the contribution of the Bragg peaks is left. It can be concluded that an amorphous intermediate structure forms before crystallization starts and is consumed later by the growing crystals. Evolution and kinetics of the two components can be followed in real-time by X-ray scattering and microscopy.

CPP 4.5 Mon 10:30 ZEU 114

Growth of nanoparticles - from milliseconds to hours — ●TORBEN SCHINDLER, MARTIN SCHMIELE, TILO SCHMUTZLER, THAER KASSAR, and TOBIAS UNRUH — Lehrstuhl für Kristallographie und Strukturphysik, Friedrich-Alexander-Universität Erlangen Nürnberg, Staudtstr. 3, 91058 Erlangen

Zinc oxide is a promising semiconductor material, which shows interesting optical and electronic properties on the nanoscale and makes it a promising candidate for many applications, e.g. solar cells. However, detailed knowledge about the kinetics of nucleation and growth of the nanoparticles is crucial for a targeted production.

The nanoparticles are synthesized by simply mixing a precursor and an alkaline solution. The growth of the nanoparticles can be studied using in-situ time-resolved small angle X-ray scattering (SAXS). A stopped flow device at a synchrotron SAXS instrument enabled us to determine the size of the nanoparticles as early as 5 ms after the synthesis, with which we could detect a strong increase of the particle diameter especially within the first 200 ms. In addition, an unexpected behavior was observed using triethylamine as alkaline solution. The particle diameters are fluctuating on a ms-timescale during the ripening process. These findings will be presented with additional absorption spectroscopy studies to describe the time- and temperature-dependent ripening process of differently synthesized ZnO nanoparticles from milliseconds to hours.

CPP 4.6 Mon 10:45 ZEU 114

Triply-intergrown distorted ths nets: A new tricontinuous equilibrium morphology in copolymeric systems — ●MICHAEL G. FISCHER^{1,2}, LILIANA DE CAMPO², STEPHEN T. HYDE², and GERD E. SCHROEDER-TURK¹ — ¹Institut für Theoretische Physik I, Friedrich-Alexander Universität Erlangen-Nuernberg, Staudtstr. 7, 91058 Erlangen, Germany — ²Dept. of Applied Mathematics, Research School

of Physics and Engineering, The Australian National University, Canberra ACT 0200, Australia

Copolymeric self-assembly provides an efficient route to the formation of ordered 3D nanostructures. The most complex equilibrium structure in diblock copolymer melts is the core-shell Gyroid based on the intergrowth of two continuous network domains. Adaption of the molecular architecture is a strategy to achieve different phases, such as kaleidoscopic columnar phases in star-shaped triblock terpolymers. However, the formation of phases based on more than 2 network domains has not yet been reported in copolymer melts. We show that a triply-periodic tricontinuous structure based on the intergrowth of three nets is a stable equilibrium phase of star-shaped triblock copolymers when an extended core is introduced into the molecules. We use self-consistent field theory to confirm the geometric intuitions why the introduction of the core leads to the formation of this new phase. Its effect is a change in the relative importance of interface tension between the three polymeric species and entropic chain stretching to the free energy. This phase is the first tricontinuous network phase in copolymer melts, which has long-range crystalline order but low symmetry.

15 min. break

CPP 4.7 Mon 11:15 ZEU 114

An in situ GISAXS study of BCP thin films during annealing in neutral and in selective solvent vapors — ●ILJA GUNKEL^{1,2}, XIAODAN GU², ALEXANDER HEXEMER¹, and THOMAS RUSSELL² — ¹Lawrence Berkeley National Laboratory, Berkeley, USA — ²University of Massachusetts, Amherst, USA

Solvent vapor annealing (SVA) is a means to achieve lateral order of block copolymer (BCP) microdomains in thin films but the underlying mechanism of the ordering process is ill-understood. Here, we used real time in situ grazing-incidence small-angle x-ray scattering (in situ GISAXS) to investigate the ordering of BCP microdomains as solvent vapor was added or removed. We systematically studied the influence of the amount of swelling and solvent removal rate on the lateral order of BCP microdomains in neutral and selective solvent vapors, respectively. In case of neutral solvent vapor larger grain sizes were observed at higher swelling while for selective solvent vapor high swelling induced changes in the packing of microdomains. The effect of solvent removal on the degree of lateral order was studied by deswelling films at different removal rates. Here, we observed a substantial deterioration of lateral order of microdomains in selective solvent vapor that is significantly stronger than in neutral solvent vapors, where the fastest solvent removal rate even allowed to freeze in the ordered microdomain structure of the swollen BCP film.

CPP 4.8 Mon 11:30 ZEU 114

Influencing molecular thin film growth with light — ●LINUS PITHAN¹, HANNES ZSCHIESCHE¹, ANTON ZYKOV¹, CHRISTOPHER WEBER¹, SEBASTIAN BOMMEL², and STEFAN KOWARIK¹ — ¹Humboldt Universität, Fachbereich Physik, Berlin — ²DESY, Hamburg

The possibilities to control the orientation and structure of molecular thin films during growth are limited to very few degrees of freedom e.g. the substrate temperature and molecular deposition rate. Here we show that light can influence the molecular growth.

Vacuum deposited α -sexithiophene (α -6T) films (OMBE) tend to grow in different crystal structures. Most prominent are the low temperature (LT) and high temperature (HT) polymorphous. Both structures are found to coexist when KCl is used as substrate material, as observed by real-time x-ray diffraction studies. Using light illumination during growth we show that the coexistence can be controlled and the phase purity can be increased by eliminating the HT phase. This demonstrates the possibility to use laser illumination as new control parameter to influence organic molecular beam deposition.

CPP 4.9 Mon 11:45 ZEU 114

Switchable Properties of Smart Coatings from Polymeric Micelles Triggered by External Stimuli — ●INNA DEWALD¹, JULIA GENSEL¹, JOHANN ERATH¹, EVA BETTHAUSEN², AXEL H. E. MÜLLER^{2,3}, and ANDREAS FERY¹ — ¹University of Bayreuth, Physical Chemistry II, Germany — ²University of Bayreuth, Macromolecular Chemistry II, Germany — ³Johannes Gutenberg University Mainz, Institute of Organic Chemistry, Germany

Today, many objects of our everyday life consist of coated materials indicating their growing importance in the modern era of technology.

Following this trend in recent years, formation of a variety of smart coatings using macromolecular building blocks has been demonstrated. On that account, we investigate the potential of pH-sensitive ABC triblock terpolymer micelles. The use of such colloidal particles as base material for thin films has several advantages from a material-science perspective, e.g. these building blocks can be stimulus-responsive and multi-functional on the single particle level, while coatings can be formed by simple physisorption. Using the LbL approach for pH-responsive micelles leads to coatings with novel properties, internal hierarchy and collective stimulus response of the integrated nanostructures.[1] In our work, we investigate the effects of pH on surface properties of these films [2] and explore their potential for applications as active surfaces for self-regulated bacteria release which change their surface characteristics in response to cellular metabolism.[3] 1. Gensel J. et al., Chem. Sci., 2013, 4, 325-334. 2. Gensel J. et al., Soft Matter, 2011, 7, 11144-11153. 3. Gensel J. et al., Adv. Mater., 2012, 24, 985-989.

CPP 4.10 Mon 12:00 ZEU 114

In-situ PDF study of Precursor Formation and Nucleation of ZnO Nanoparticles — ●MIRIJAM ZOBEL and REINHARD B. NEDER — Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen-Nürnberg

Most semiconductor nanoparticles are produced in sol-gel processes. For the model system zinc oxide (ZnO), abundant different synthesis strategies exist, often in organic solvents. Though the final crystalline nanoparticles are well characterized, little is known about the evolution of the crystallinity of the precursors and nanoparticles in solution. Using high-energy synchrotron radiation, we can study such nucleation processes in-situ with a 20 s time resolution, even at very low concen-

trations of 30 mM. To our knowledge, this is the first study of this kind. Fourier transformation of the scattering data provides us with pair distribution functions (PDF). Those mirror the distribution of interatomic distances within the sample and allow the derivation of different nanoparticle properties such as size, shape and crystallinity. Firstly, after base addition we observe metastable precursors of about 1 nm in diameter. Compared with the final wurtzite crystal structure, the PDF of the precursors show broadened peaks of the next-neighbour distances. This indicates precursor structures which possess local domains of both tetrahedral as well as octahedral arrangement. After a lag time of 100 min those precursors spontaneously nucleate to 2 nm particles, which further grow with time. We show this nucleation and growth behavior by multiphase fits of the PDFs and structural modelling of the precursor and nanoparticles.

CPP 4.11 Mon 12:15 ZEU 114

Computer simulation of heterogeneous nucleation on curved surfaces — ●HENNING HÖRSTERMANN, JULIA KUNDIN, and HEIKE EMMERICH — Materials and Process Simulation, University of Bayreuth, Germany

We show how the combination of string method with the phase-field approach can be extended from simulations of homogeneous nucleation to heterogeneous nucleation. From these simulations, it is possible to directly obtain nucleation barriers for heterogeneous nucleation on arbitrary surfaces as well as information about the size and shape of the critical nucleus. We test the method by comparing the dependence of the nucleation barrier for heterogeneous nucleation on concave and convex surfaces on the surface curvature obtained from three-dimensional phase-field simulations with predictions from classical nucleation theory and find good agreement between them.

CPP 5: Energy Materials: Water Splitting, Batteries, and Supercapacitors (original: HL, joined by CPP)

Time: Monday 10:45–12:30

Location: POT 081

CPP 5.1 Mon 10:45 POT 081

Highly efficient photocatalytic water splitting with colloidal CdS nanorods by mediated hole scavenging — ●THOMAS SIMON, AURORA MANZI, CHRISTIAN WOLFF, JACEK STOLARCZYK, and JOCHEN FELDMANN — Photonics and Optoelectronics Group, Ludwig-Maximilians-Universität München, Amalienstr. 54, D-80799

Solar hydrogen production is considered to be as one of the biggest challenges for future energy supply. Colloidal semiconductor nanoparticles, as sunlight absorber with additional noble metal nanoparticles as hydrogen catalyst are well known for photocatalytic hydrogen generation. Many of these systems suffer from low solar to hydrogen efficiencies unless high cost and rare materials like platinum or ruthenium compounds are used as co-catalysts. We demonstrate that it is possible to overcome all these problems with CdS nanorods with a very simple earth-abundant nickel-based co-catalyst. An apparent quantum yield exceeding 50% and long term stability of more than 200h could be achieved. We show that the photocatalytic activity is enhanced ten-fold in highly alkaline environment. Thanks to favourable band alignment the hydroxide anion acts as a redox shuttle relaying the hole from the nanocrystals. Since the hole transfer is considered to be the limiting factor, the quick hole scavenging at high pH is responsible for the enhancement of photocatalytic hydrogen evolution. [1]

[1] T. Simon, M.J. Berr, A. Vaneski, D. Volbers, R. Wyrwich, M. Döblinger, A.S. Susha, A.L. Rogach, F. Jäckel, J.K. Stolarczyk, J. Feldmann, submitted

CPP 5.2 Mon 11:00 POT 081

Three-dimensional Ordered Macro-mesoporous Mo:BiVO₄ Photoelectrode toward Efficient Photoelectrochemical Water Splitting — ●MIN ZHOU^{1,2}, YANG XU¹, CHENGLIANG WANG¹, LIAOYONG WEN¹, YONG LEI¹, and YI XIE² — ¹Ilmenau University of Technology, Institute of Physics & IMN MacroNano (ZIK) Prof. Schmidt-Str. 26, 98693 Ilmenau, Germany — ²University of Science & Technology of China, Hefei, China

In view of the worldwide energy challenge in the 21st century, the technology of semiconductor-based photoelectrochemical (PEC) water splitting has received considerable attention as an alternative approach for solar energy harvesting and storage. BiVO₄ has been regarded as

a promising material for PEC water splitting, but it suffers from a major challenge on charge migration. In order to meet this challenge, for the first time, we design a three-dimensional(3D) ordered macroporous architecture of Mo:BiVO₄ through a controllable colloidal crystal template method. Within expectation, a superior photocurrent density is achieved in return for this design. This enhancement originates primarily from effective charge migration according to the analysis of electrochemical impedance spectroscopy. All the results highlight the great significance of the 3D ordered macro-mesoporous architecture as a promising photoelectrode model for the application in solar conversion. The cooperating amplification effects of nanoengineering from composition regulation and morphology innovation provide new opportunities for creating more purpose-designed photoelectrodes with highly efficient performance.

CPP 5.3 Mon 11:15 POT 081

Three-dimensional Composite Aerogels and Other Nanostructures for Improved Electrochemical Property — ●LIYING LIANG^{1,2}, YIMENG XU¹, HAIMEI LIU¹, and YONG LEI² — ¹Beijing University of Chemical Technology, State Key Laboratory of Chemical Resource Engineering, 100029 Beijing (PR China) — ²Ilmenau University of Technology, Institute of Physics & IMN MacroNano (ZIK) Prof. Schmidt-Str. 26, 98693 Ilmenau (Germany)

Three-dimensional (3D) graphene aerogels possess a lot of unique properties, such as light weight, high conductivity, large surface area, high mechanical strength, and ample volume with hierarchically porous structure, which make them widely applied in various technological fields. Here, 3D porous composite aerogels have been synthesized via an innovative in situ hydrothermal method assisted by freeze-drying process. In this hybrid structure, one-dimensional (1D) AgVO₃ nanowires are uniformly dispersed on two-dimensional (2D) graphene nanosheets surfaces or penetrate through the graphene sheets, forming 3D porous composite aerogels. The composite aerogels as cathode materials for lithium-ion batteries, exhibit high discharge capacity, excellent rate capability, and good cycling stability. We are also preparing more novel nanostructures by using AAO templates, which are expected to provide excellent electrochemical performance.

CPP 5.4 Mon 11:30 POT 081

Three-dimensional Metal Oxides Based Nano-arrays Anodes for Sodium Ion Batteries — •YANG XU, MIN ZHOU, HUAPING ZHAO, CHENGLIANG WANG, and YONG LEI — Institute of Physics, Ilmenau University of Technology, 98693 Ilmenau, Germany,

The discovery of new materials/microstructures for electrodes in sodium ion batteries (NIBs) is receiving high levels of scientific attention, as sodium is substantially less expensive and more abundant than lithium. However, there is a limited choice of electrode materials that are suitable hosts to accommodate Na ions and allow for reversible insertion/extraction reactions, since Na ions are 55% larger in radius than Li ions. Of those, most have been identified to be potentially useful as cathodes. On the anode side, hard carbonaceous materials and insertion of Sn, Sb, Pb, and their alloys based anodes have been demonstrated to be highly promising. Another emerging class of materials that remains relatively unexplored in this case is conversion and/or insertion electrodes using transition metal oxides with reasonably low insertion potential. We report the successful utilization combining the nano-structured transition metal oxides and three-dimensional metallic current collector for NIBs anodes, and the results are demonstrated to be promising: the electrodes exhibited a highly stable reversible charge storage capacity over long term cycling, and were able to withstand high rate cycling with fully recovering the initial capacity. This proof-of-principle demonstration opens a way forward for future work on nano-architectures with better NIBs anode performance.

CPP 5.5 Mon 11:45 POT 081

First principles study on the electronic properties of NaO₂ — •MARKUS HEINEMANN¹, PASCAL HARTMANN², CONRAD L. BENDER², PHILIPP ADELHELM², JÜRGEN JANEK², and CHRISTIAN HEILIGER¹ — ¹I. Physikalisches Institut, Justus Liebig University, 35392 Giessen, Germany — ²Physikalisch-Chemisches Institut, Justus Liebig University, 35392 Giessen, Germany

In the light of the recent discovery of rechargeable room-temperature sodium superoxide (NaO₂) batteries [1], a deeper understanding of the electronic properties of NaO₂ has become of broad interest. We investigate the electronic structure of NaO₂ using the framework of density functional theory and employ a hybrid functional approach for the exchange and correlation interaction. The disordered pyrite structure of the NaO₂ room-temperature phase is modeled by taking into account various superoxide orientations in our computations. Our band structure calculations indicate that NaO₂ is an insulator with an energy band gap in the range of 2 eV and that different superoxide alignments lead to a broadening of the conduction band. We compare our calculations to recent experimental investigations on the conductivity of NaO₂.

[1] P. Hartmann, C. L. Bender, M. Vračar, A. K. Dürr, A. Garsuch, J. Janek, and P. Adelhelm, *Nature Mat.* 3486, 1 (2012)

CPP 5.6 Mon 12:00 POT 081

Photostability of GaN-metal interfaces in aqueous media — •CARINA EHRIG^{1,2}, RALF KRAUSE¹, CHRISTOPH BRABEC², and GÜNTER SCHMID¹ — ¹Siemens AG, CT RTC MAT IEC-DE, Erlangen — ²Lehrstuhl für Werkstoffe der Elektronik- und Energietechnik, FAU Erlangen-Nürnberg, Erlangen

Gallium nitride (GaN) is a well-established semiconductor in optoelectronic applications. It has a wide band gap of 3.4 eV and is thus excitable in the near UV range. A promising application of GaN is its use as a photo electrode driving electrochemical reactions such as photocatalytic water splitting for generation of hydrogen without consumption of fossil fuel or emission of CO₂. The corrosion resistance of those photo electrodes in aqueous media is one of the main factors determining their lifetimes and thus plays an important role for their applicability for highly efficient solar energy conversion. It has been demonstrated in photocatalytic experiments, that under UV-illumination n-type GaN acts as oxygen evolving photo anode and p-type GaN as hydrogen evolving photo cathode.

In the present work, the corrosion resistance of metal-coated n-GaN and p-GaN photoelectrodes in aqueous media is investigated by electrochemical measurements. The influence of an externally applied potential under light excitation as well as the effect of long-term photo-induced stress are studied. It is observed that without illumination the GaN surfaces and GaN-metal interfaces are rather stable, whereas they undergo different corrosion processes when exposed to UV light.

CPP 5.7 Mon 12:15 POT 081

Growth and characterization of 3D graphene networks for supercapacitors — •SIMON DRIESCHNER and JOSE ANTONIO GARRIDO — Walter Schottky Institut, TU München, Am Coulombwall 4, 85748 Garching

The use of graphene as electrode material in supercapacitors has drawn great interest due to a suitable combination of material properties like high surface to volume ratio, high conductivity, and chemical stability. Since the capacitance of one single graphene sheet is rather limited, a continuous 3D network of graphene is expected to enhance the performance of graphene-based supercapacitors. We demonstrate the growth of 3D graphene by chemical vapor deposition (CVD) using a nickel foam as scaffold and a wet-etching transfer, yielding a free-standing macroporous graphene network of high crystalline quality, as shown by Raman spectroscopy. Cyclic voltammetry, charge-discharge measurements, and electrochemical impedance spectroscopy are used to assess the potential of 3D networks of CVD graphene for energy storage applications. We also compare the electronic double layer capacitance of bare graphene foam to the pseudo-capacitance introduced by conductive polymers.

CPP 6: Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale (original: O, joined by CPP)

Non-equilibrium processes such as charge and heat transport are central to electronic and thermoelectric applications. Understanding these phenomena at the nanoscale challenges both theory and experiment. Basic theoretical issues are related to the role of quantum mechanics, the interplay of ballistic, diffusion and hopping processes, the importance of dissipation, the effect of electronic correlation, and the signatures of unusual quantum states. On the experimental side devising measurements to unravel these phenomena in a controlled way poses severe difficulties. In this regard, optical lattices of cold atoms are emerging as a powerful laboratory to test theoretical models and discover unforeseen phenomena.

This symposium will cover current issues in the field by bringing together scientists working in different specific areas with the aim of fostering interdisciplinary discussion, assessing current theoretical understanding, and indicating future goals with emphasis on electronic structure theory.

Organizers: Roberto Car (Princeton), Kristian S. Thygesen (Lyngby) and Matthias Scheffler (Berlin)

Time: Monday 10:30–13:15

Location: TRE Ma

Topical Talk

CPP 6.1 Mon 10:30 TRE Ma

Molecular junction transport: some theoretical and computational considerations — •MARK RATNER¹ and MATTHEW REUTER² — ¹Chemistry, Northwestern University, Evanston Illinois 60208 USA — ²Chemistry, Northwestern University, Evanston Illinois 60208 USA

Following the development of break junction techniques, and very elegant measurements by many labs worldwide, the understanding of the community for single molecule transport junctions on the experimental side has been very nicely unified. While there are still challenges, interpretations of the transport (and indeed of some second-order response

properties) is now quite sophisticated.

There have been major advances in the computational approaches also, and in many cases, computations and measurements can be compared quantitatively. But there are some remaining difficulties in the computational and theoretical approaches, and this talk will discuss a few of them.

The topics addressed will be: single molecule aspects, histograms and their usage, time-dependence of the transport, and ghost transmission and computational accuracy.

CPP 6.2 Mon 11:00 TRE Ma

On the description of biased nanocontacts from ab initio — ●STEVEN ACHILLES¹, JÜRGEN HENK¹, MICHAEL CZERNER², CHRISTIAN HEILIGER², and INGRID MERTIG¹ — ¹Institute of Physics, Martin Luther University Halle-Wittenberg, D-06099 Halle, Germany — ²I. Physikalisches Institut, Justus Liebig University, D-35392 Giessen, Germany

A suitable description of arbitrary shaped and biased nanocontacts is very important for investigating and predicting physical effects of materials on the nanometer scale. In particular, the electronic transport properties under finite bias voltages are of great interest.

To account for systems under finite bias we extended our Korringa-Kohn-Rostoker Green's function method [1] to the Keldysh formalism [2]. The method was developed for different types of geometries, i.e. planar junctions [3] and embedded real-space clusters [4]. Both implementations include a self-consistent treatment of the electronic structure under external bias using the nonequilibrium density.

We present ab initio results of voltage drops, the charge relaxation under finite bias voltage and current-voltage characteristics for different types of geometries.

[1] R. Zeller, P.H. Dederichs, B. Ujfalussy, L. Szunyogh, and P. Weinberger, Phys. Rev. B 52, 8807 (1995); P. Zahn, I. Mertig, R. Zeller, and P.H. Dederichs, Mat. Res. Soc. Symp. Proc. 475, 525 (1997).

[2] L.V. Keldysh, Sov. Phys. JETP 20 (4), 1018-1026 (1965).

[3] S. Achilles et al., Phys. Rev. B 88 (12), 125411 (2013).

[4] S. Achilles et al., to be published

CPP 6.3 Mon 11:15 TRE Ma

Elasticity changes in molecular junctions under bias: an ab-initio study — ●CLOTILDE S. CUCINOTTA¹, MELIN BAI^{1,2}, IVAN RUNGGER¹, SHMIN HOU², and STEFANO SANVITO¹ — ¹School of Physics and CRANN, Trinity College Dublin, College Green, Dublin 2, Ireland — ²Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, China

Non-conservative current induced forces are at the origin of a rich variety of dynamical processes, including vibrations, rotations, phonon energy flow, desorption and reactions. The ability to simulate these phenomena paves the way for crucial advances in interface physics and in molecular electronics. New insights into how the presence of non-conservative forces can affect the vibrational spectrum of prototypic Au-H₂-Au nano-junctions are obtained by the Non Equilibrium Green Functions approach combined with Density Functional Theory as implemented in the Smeagol code [1]. The modification of the phonon spectrum of the junction in the presence of an external bias is for the first time analysed, in terms of charge redistribution caused by the electron flow, potential drop and differences in an average distance collective variable. Phonon modes changes are related to a change in bias of some of the elastic constants. The importance of electric field vs. current effects is compared. The elasticity changes of the molecular junction with bias are interpreted in terms of the current flowing through the system. [1] <http://www.smeagol.tcd.ie/SmeagolDownloads.htm>.

CPP 6.4 Mon 11:30 TRE Ma

Carbon nanotubes decorated with magnetic clusters: magnetism, electron transport and gas sensing — ●ZEILA ZANOLLI¹ and JEAN-CHRISTOPHE CHARLIER² — ¹Forschungszentrum Juelich, PGI and IAS, Juelich, Germany — ²IMCN, Université catholique de Louvain (UCL), Belgium

In this work, first-principles techniques and non-equilibrium Green's function approaches are used to investigate magnetism and spin-polarized quantum transport in carbon nanotubes (CNTs) decorated with transition metal magnetic nanoclusters (NC).

For small cluster sizes (< 1 nm), *ab initio* calculations predict a considerable local magnetic moment that induces spin polarization in the host CNT due to a strong mutual interaction with the magnetic NC. Such a huge local magnetic perturbation can be tailored by molecular

adsorption on the metallic NC, thus modifying both the magnetization and the spin-dependent conductance of the hybrid CNT-NC system. The adsorption of benzene on Ni- or Pt-decorated metallic CNTs has been investigated as a test case. The ab initio simulations demonstrate that the magnetization change due to the absorption of a single C₆H₆ molecule should be large enough to be detected experimentally using either magnetic-AFM or SQUID magnetometer. Consequently, the present research suggests a novel approach for single molecule gas detection, based on local magnetic moment measurements in CNT-NC hybrid systems [1].

[1] Z. Zanolli, J.-C. Charlier, ACSnano 6 (2012) 10786-10791.

15 min. break

Topical Talk

CPP 6.5 Mon 12:00 TRE Ma

Insight into Charge Transport in Molecular Junctions from Ab Initio Theories of Level Alignment — ●JEFFREY B. NEATON — Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA, USA — Department of Physics, University of California, Berkeley, Berkeley, CA — Kavli Energy Nanosciences Institute, Berkeley, CA

Recent scanning tunneling microscope-based break-junction experiments of molecular junctions – devices formed by trapping organic molecules between macroscopic metallic electrodes – have reported robust conductance, thermopower, switching behavior, quantum interference effects, spin-filtering phenomena, and even nonlinear effects such as rectification, establishing such junctions as unique and revealing windows into the physics of charge transport at the molecular scale. In this talk, I will summarize a predictive approach to compute and understand the transport properties of molecular junctions with good accuracy. Our approach includes important exchange and correlation effects missing in standard DFT Kohn-Sham junction level alignment, building on self-energy corrections within a GW approximation. Advantages and limitations of our approach will be discussed quantitatively in the context of a direct comparison with recent photoemission and transport measurements. I will also describe applications of this approach to select junctions exhibiting novel trends in conductance, thermopower, and nonlinear IV characteristics, where new physical insight is obtained by relating computed transport phenomena to junction structure and chemistry.

CPP 6.6 Mon 12:30 TRE Ma

Towards First-Principles Modeling of Solvent Effects in Photo-Catalytic Water Splitting — ●STEFAN RINGE, HARALD OBERHOFER, SEBASTIAN MATERA, and KARSTEN REUTER — Technische Universität München, Germany

In the context of solar energy conversion the search for new materials for photo-catalytic water splitting has received new impetus. While in general powerful, computational screening approaches are struggling with the complexity of the underlying physical processes at the solid-liquid interface. Recent work points in particular at the necessity to include at least an efficient description of solvent screening effects to compute meaningful descriptors even in simple computational hydrogen electrode approaches. To this end, we present an implementation of the modified Poisson-Boltzmann (MPB) implicit solvation model in the highly parallel and numerically efficient all-electron DFT code FHI-aims. Optimally integrating into this code environment, we solve the MPB equation in a novel approach based on an expansion of the electrostatic potential in the localized basis functions of FHI-aims. In contrast to common numerical multi-grid solvers this approach can directly make use of the optimized integration schemes used to reach self-consistency and removes the need for numerical interpolation between different grids. We demonstrate the approach and its efficiency for a range of molecular test systems, and show first results for catalytic water splitting on gold nano-clusters.

CPP 6.7 Mon 12:45 TRE Ma

Towards a combined QM/MM and implicit solvent description of photoelectrochemical processes — ●MARKUS SINSTEIN¹, DANIEL BERGER¹, RAN JIA², VOLKER BLUM³, HARALD OBERHOFER¹, and KARSTEN REUTER¹ — ¹Technische Universität München, Germany — ²Jilin University, P.R. China — ³Duke University, USA

Photoelectrochemical systems are widely explored to drive energy-relevant redox reactions like water splitting or CO₂ reduction. The detailed analysis of the involved elementary processes via first-principles calculations is challenged by the necessity to simultaneously account

for the extended semiconductor photocatalyst and the liquid electrolyte. Especially for charge (proton and/or electron) transfer steps traditionally employed periodic boundary condition approaches involve charged supercells with difficult to control finite size errors. To this end, we present a solid state QM/MM embedding approach, in which only a finite cluster model of the photocatalyst surface is treated quantum mechanically and the correct Madelung potential of the periodic system is obtained by embedding into a charge field. For the efficient modeling of photoelectrochemical processes we combine this approach with an implicit solvation scheme within the DFT package FHI-aims. Finally, we also show early test results of the combined QM/MM implicit solvent model.

CPP 6.8 Mon 13:00 TRE Ma

Ab-initio Simulation of Molecular Networks on the Surface of Water — ●RALPH KOITZ, MARCELLA IANNUZZI, ARI P SEITSONEN, and JÜRIG HUTTER — University of Zurich, Zurich, Switzerland

Molecules adsorbed on surfaces play an important role in catalysis, sur-

face science, and nanotechnology. Traditionally, research has focused on various adsorbates atop metals and metal oxides using computational and surface-science techniques. More recently, however, it was demonstrated that ordered monolayer networks can also be formed on the surface of liquid water by using metal ions to bind together multidentate precursor molecules. As these assemblies are difficult to characterize, computational methods can provide valuable insight into their formation and structure.

In this contribution we present large-scale DFT-based molecular dynamics simulations of the formation of a network of *tris*-terpyridine-derived molecules (TTPB) on a water slab. In particular, we focus on the structure of the molecule on the surface, the mechanism of Zn^{2+} ion insertion from the solution and the subsequent linking of molecules into aggregates. We employ the metadynamics method to quantify the free energy surface of the involved processes. Our results provide detailed insight into on-surface and subsurface diffusion in this system and chemical reactions of TTPB on the surface of water.

CPP 7: Invited Talk by Martin Fally: Optics with Neutrons using Holographic Gratings (original: DF, joined by CPP, TT, KR)

Time: Monday 9:30–10:15

Location: GER 37

Invited Talk

CPP 7.1 Mon 9:30 GER 37

Optics with neutrons using holographic gratings — ●MARTIN FALLY¹, JÜRGEN KLEPP¹, CHRISTIAN PRUNER², and YASUO TOMITA³ — ¹Faculty of Physics, Uni Wien, Austria — ²Department of Materials Science and Physics, Uni Salzburg, Austria — ³University of Electro-Communications, Tokyo, Japan

All neutron-optical phenomena are governed by the neutron-optical potential or, equivalently, the neutron refractive-index. Thus, an important task in the design of neutron-optical elements is to efficiently pattern the neutron refractive-index of materials. For this purpose we use light-sensitive materials and employ holographic techniques to produce diffraction gratings for neutrons.

After an introduction to the basics of neutron optics and the chal-

lenges as compared to light optics I will discuss our recent experiments, where we successfully demonstrated the power of this approach. Two- and three-port beam-splitters as well as free-standing film mirrors for cold and very-cold neutrons were set up by exploiting the Pendellösung interference effect. Another intriguing possibility is offered by holographic gratings containing superparamagnetic nanoparticles to produce business card-size neutron polarizers working in comparably low external magnetic induction. Such devices are being developed at present. Finally, I will give an outlook on novel neutron-scattering instrumentation and techniques which are expected from those advancements.

In collaboration with: I. Drevensek-Olenik, S. Gyergyek, J. Kohlbrecher, P. Geltenbort, R. A. Rupp

CPP 8: Organic Electronics and Photovoltaics (joint session with DS/HL/O) II

Simulations, Polymers, Solar Cells

Time: Monday 15:00–18:00

Location: ZEU 222

CPP 8.1 Mon 15:00 ZEU 222

Quantumchemical Calculation of Zn-Porphyrine-Indolocarbazole-Conjugates — ●KSENIA KORSHUNOVA and WICHARD J. D. BEENKEN — Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany

We have investigated the structure of Zn-porphyrin-indolocarbazole conjugates with a different number of indolocarbazole meso-substituents without and with THF and DMF axial ligands by quantumchemical methods in order to interpret experimental data such as Absorption spectra, fluorescence lifetime and quantum yields in different solutions. Contrarily to our expectations, we found very weak deformation of the Zn-porphyrin macrocycle under the influence of axial THF and DMF ligands, which only tend to pull the central Zn-atom out of its equilibrium position in the macrocycle plane. This means that the very different fluorescence yields for Zn-porphyrin-indolocarbazoles in toluene, THF, and DMF cannot be explained by a conformational change.

CPP 8.2 Mon 15:15 ZEU 222

Estimating Coulomb model parameters in organic molecules from first principles — ●IRINA PETRESKA^{1,2}, LJUPCO PEJOV², LJUPCO KOCAREV^{3,4}, and GERTRUD ZWICKNAGL¹ — ¹Institut für Mathematische Physik, Technische Universität Braunschweig, 38 106 Braunschweig, Germany — ²Faculty of Natural Sciences and Mathematics, Ss. Cyril and Methodius University, 1 000 Skopje, Republic of Macedonia — ³Macedonian Academy of Sciences and Arts, Skopje, Republic of Macedonia — ⁴Faculty of Computer Science and Engineering, Ss. Cyril and Methodius University, 1 000 Skopje, Republic of Macedonia

The Coulomb parameters are estimated from electronic structure calculations based on Density Functional Theory (DFT). Of particular interest are phenylene ethynylene oligomers exhibiting electric-field controlled conductance switching. The charge transport properties are analyzed adopting a simplified two-site model accounting for Coulomb correlation effects. The Coulomb parameters are deduced from a population analysis. The DFT calculations employ a combination of the Becke's three parameter adiabatic connection exchange functional (B3) with the Lee-Yang-Parr correlation one (LYP). The Kohn-Sham SCF equations are iteratively solved using the LANL2DZ basis set, for orbital expansion, on an "ultrafine" grid for numerical integration.

CPP 8.3 Mon 15:30 ZEU 222

Theoretical Study of Simultaneous Electron- and Excitation Energy Transfer in a Fullerene-Chromophore Complex — ●THOMAS PLEHN, JÖRG MEGOW, and VOLKHARD MAY — Humboldt-Universität zu Berlin, Germany

Mainly during the last decade fullerene based molecular systems have been of increasing interest with regard to future components in dye sensitized solar cells and artificial photosynthetic systems. This theoretical study focuses on the characteristic photoinduced charge separation process in a supramolecular complex containing a single fullerene and six pyropheophorbide-a molecules. For this purpose the excitation energy transfer processes are treated among the six chromophores. Simultaneously electron transfer takes place from the excited chromophores to the fullerene. The whole investigation uses molecular dynamics simulations of the highly flexible complex in explicit solvent environment. The transfer phenomena are described in terms of a special mixed

quantum-classical version of the Förster- [1] and the well-known classical Marcus rate. Finally the charge separation process is computed concerning an ensemble of complexes. The resulting dynamics are in very good agreement with appropriate experimental data [2].

[1] J. Megow et al., *ChemPhysChem* 2011, 12 645-656

[2] M. Regehy et al., *J. Phys. Chem. B* 2007, 111, 998

Invited Talk

CPP 8.4 Mon 15:45 ZEU 222

Controlled crystallization of semiconducting polymer thin films — ●SABINE LUDWIGS — Institute for Polymer Chemistry, University of Stuttgart, Germany

The talk will give an overview over current activities in my team on the morphological control of semiconducting polymers for applications in polymer electronics. Different methods to induce and control crystalline order over large areas in thin films will be presented. These include swelling and deswelling in defined solvent vapour atmospheres of good solvents and crystallization under confinement and with external fields. Regarding polymer materials we are currently extending our studies from conventional p-type semiconductors based on pure thiophenes like P3HT[1] to high performance p-type low bandgap polymers such as PCPDTBT[2] and n-type polymers such as PNDI2OD-2T[3]. The control of molecular orientation over macroscopic distances allows us to study the relationship between the polymer microstructure and the resulting charge transport properties along specific crystallographic directions.

[1] E. Crossland, K. Tremel, F.S.U. Fischer, K. Rahimi, G. Reiter, U. Steiner, S. Ludwigs, *Adv. Mater.* 2012, 24, 838. [2] F.S.U. Fischer, K. Tremel, A.-K. Saur, S. Link, N. Kayunkid, M. Brinkmann, D. Herrero-Carvajal, J. T. López Navarrete, M. C. Ruiz Delgado, S. Ludwigs, *Macromolecules* 2013, 46, 4924. [3] K. Tremel, F.S.U. Fischer, N. Kayunkid, R. DiPietro, R. Tkachov, A. Kiriy, D. Neher, S. Ludwigs, M. Brinkmann, Charge Transport Anisotropy in Highly Oriented Thin Films of the Acceptor Polymer P(NDI2OD-T2), submitted.

15 min break

CPP 8.5 Mon 16:30 ZEU 222

Conjugated oligomers near surfaces with different physical and chemical nature: MD simulation of adsorption layers — ●OLGA GUSKOVA¹ and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, D-01069 Dresden — ²Technische Universität Dresden, Institut für Theoretische Physik, Zellescher Weg 17, D-01062 Dresden

Atomistic molecular dynamics simulations are used to explore some general principles of 2D supramolecular organization of conjugated oligomers on adsorbing substrates. Two systems are studied: (i) terminally substituted dicyanovinyl quaterthiophenes, prototypic absorbers for small molecule organic solar cells on a silica surface [1] and (ii) 2,5-dialkoxy-phenylene-thienylene-based oligomers on epitaxial monolayer graphene [2]. We demonstrate that the driving force of molecular orientation on substrate is embodied by the chemical nature of the surface and the character and position of functional groups of the conjugated molecule bearing, i.e. the underlying balance of forces defines the spatial orientation - standing upright or lying-down molecules on substrates. This force balance clearly allows isolated molecules to explore flat, bent or twisted molecular conformations and to exploit force anisotropies to maximize their interactions when crystals are growing.

[1] O.A. Guskova et al. // *J. Phys. Chem. C* 2013. V. 117. P. 17285.

[2] R. Shokri et al. // *J. Am. Chem. Soc.* 2013. V. 135. P. 5693.

CPP 8.6 Mon 16:45 ZEU 222

Frank elastic constants in nematic mesophases of polymeric semiconductors — ●PATRICK GEMÜNDE, KURT KREMER, and KOSTAS CH. DAOULAS — Max Planck Institute for Polymer Research, Mainz

Liquid crystalline (LC) mesophases of polymeric semiconductors[1] can facilitate material processing. We develop a particle-based modeling approach considering poly(alkylthiophenes) as a test system for studying nematic mesophases. The method uses "soft tube" representations of chains where non-bonded potentials are defined by soft, directional interactions.[2,3] Here, we focus on Frank elastic constants (FC). Calculating FCs is important for comparing material properties from the soft model with experiments, studying theoretical questions related to FCs in polymer nematics and linking particle-based and continuum descriptions of LCs. We calculate FCs related to bend, splay and twist deformations from the fluctuations of the local nematic direc-

tor. Indeed, the magnitudes of the FCs from our simulations agree with experiments on polymer nematics. We study the dependence on system parameters, e.g. chain length, and compare with predictions by analytical field theory.[4] Eventually we study local density fluctuations in the nematic samples, which, as predicted by theory, lead to an anisotropic scattering pattern and can be related to the elastic properties.

[1] Ho et al., *Macromolecules* 43, 7895 (2010) [2] Gemünden et al., *Macromolecules* 46, 5762 (2013) [3] Daoulas et al., *J. Phys.: Condens. Matter* 24, 284121 (2012) [4] Le Doussal & Nelson, *Europhys. Lett.* 15, 161 (1991)

CPP 8.7 Mon 17:00 ZEU 222

Modeling LC mesophases in polymeric semiconductors with soft directional interactions — PATRICK GEMÜNDE, CARL POELKING, KURT KREMER, DENIS ANDRIENKO, and ●KOSTAS DAOULAS — Max Planck Institute for Polymer Research, Mainz

Often in Soft Matter mesoscale behavior couples across a hierarchy of scales to details of molecular architecture and interactions. When modeling such materials, features accounting for the latter must be included even in drastically coarse-grained (CG) representations. Focusing on liquid crystalline (LC) mesophases of polymeric semiconductors, we highlight a top-down strategy for developing such models, projecting classical density functionals on particle-based representations. Poly(3-alkylthiophenes) (P3AT) are considered as an example. Two different CG models are developed, representing: a) the polymer chain with a "soft" flexible tube [1] and b) each alkylthiophene as a plate-like object [2]. The first describes uniaxial nematics and the second captures biaxial nematic ordering, mimicking effects of anisotropy in microscopic interactions and chain architecture. We demonstrate that the model reproduces realistic material properties in nematic mesophases. In biaxial morphologies we discuss how collective orientation and planarization of molecules affects the lengths of conjugated segments, defined via conjugation-breaking torsional defects [3]. First results on the interplay between nematic ordering and phase separation in blends of P3AT with nanoparticles are presented.[1] Daoulas et al, *J. Phys.: Condens. Matter* (2012) 24, 284121 [2] Gemünden et al, *Macromolecules* (2013) 46, 5762 [3] Rühle et al, *J. Chem. Phys.* (2010) 32, 134103.

CPP 8.8 Mon 17:15 ZEU 222

Correlating structural order and morphology with transport properties in donor-acceptor block copolymers for organic photovoltaics — ●GAURAV GUPTA¹, CHETAN RAJ SINGH², RUTH LOHWASSER³, PETER MULLER BUSCHBAUM⁴, MUKUNDAN THELEKKAT³, HARALD HOPPE², and THOMAS-THURN ALBRECHT¹ — ¹Martin-Luther-Universität Halle-Wittenberg, Germany — ²Technische Universität Ilmenau, Germany — ³University of Bayreuth, Germany — ⁴Technische Universität München, Germany

Microphase separated donor-acceptor block copolymers are promising systems for morphology control in OPV's. A nanostructure on exciton diffusion length scale, crystalline order and percolating pathways for charge transport are pre-requisites for obtaining good device properties. We here present a systematic study of the correlation between structure and charge transport in thin films of P3HT-b-PPeAcr after different thermal treatments. Combining AFM, microscopy and GISAXS we show that films annealed in the melt state above the melting temperatures of both components form typical microphase separated structures oriented parallel to the substrate, while films crystallized from the disordered state as obtained from spin coating show no well-defined microphase separated structures. GIWAXS measurements reveal that crystallization from the ordered state leads to strongly textured samples. Charge carrier mobilities as measured by SCLC were improved by 2 orders of magnitude in films crystallized from the disordered state, the unfavorable orientation of the microphase morphology in melt annealed films resulted in poor device performance.

CPP 8.9 Mon 17:30 ZEU 222

Origins of Reduced Nongeminate Recombination in P3HT:PCBM Organic Solar Cells — ●MICHAEL C. HEIBER¹, JULIEN GORENFLOT¹, VLADIMIR DYAKONOV^{1,2}, and CARSTEN DEIBEL¹ — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²ZAE Bayern, 97074 Würzburg

Understanding the nongeminate recombination processes that are the dominant loss mechanisms in organic solar cells is critical to improving device performance. In P3HT:PCBM blends, nongeminate recombination has been found to be significantly slower than expected from Langevin theory and also exhibits super-second order kinetics. Several

theories for this behavior have been proposed, but a complete model has not yet been reached. To shed light on this problem, we have used a combination of transient absorption spectroscopy experiments and kinetic Monte Carlo simulations. By modeling the temperature dependence of the polaron transients measured in both neat P3HT films and annealed P3HT:PCBM blend films, we demonstrate the effects of phase separation, carrier trapping, and charge transfer states on the magnitude of the recombination rate. Furthermore, we show that while neat P3HT films exhibit second order recombination and mobility behavior indicating a Gaussian density of states (DOS), P3HT:PCBM blends are complicated by super-second order recombination that is indicative of an exponential DOS and mobility measurements that are consistent with a Gaussian DOS. To unify these observations, we show that a separate distribution of charge transfer states must be included.

CPP 8.10 Mon 17:45 ZEU 222

Model systems for interchromophoric interactions in conjugated polymer materials — ●THOMAS STANGL¹, DANIELA SCHMITZ², KLAAS REMMERSEN², DOMINIK WÜRSCH¹, FLORIAN STEINER¹, SIGURD HÖGER², JAN VOGELSANG¹, and JOHN 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 electronic aggregation between two oligomers with different well-defined distances and single polymer chains. It is concluded that the model systems can be used to investigate the impact of H-aggregation as a function of interchromophoric distance by simultaneous measurement of lifetime and single-molecule spectra. This reveals a strong heterogeneity in coupling strengths even for identical single molecules. Further, it is shown that the coupling strength varies over time on a single molecule, leading to the conclusion that electronic aggregation has to be understood as a dynamic property. In bulk polymer films, such interchromophoric coupling impacts the functionality, e.g. the emission color 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 9: Crystallization, Nucleation and Self Assembly II

Time: Monday 15:00–18:00

Location: ZEU 260

Invited Talk

CPP 9.1 Mon 15:00 ZEU 260

Self-assembly of soft colloids into meso-, para-, and quasicrystals — ●STEPHAN FOERSTER¹, ALEXANDER EXNER¹, SABINE ROSENFELDT¹, PETER LINDNER², and JAN PERLICH³ — ¹Physikalische Chemie I, Universität Bayreuth, Germany — ²Institut Laue Langevin (ILL), Grenoble, France — ³HASYLAB/DESY, Hamburg, Germany

Soft colloids interact via soft potentials and often are internally structured. At high volume fractions this leads to the formation of mesocrystals, paracrystals and quasicrystals. [1,2] We show how multi-body interactions, multiple length scales and defects decisively control self-assembly at high volume fractions. Neutron- and synchrotron X-ray diffraction are used to reveal the formation of these structures in-situ.

References: [1] S. Fischer, A. Exner, K. Zielske, J. Perlich, S. Deloudi, W. Steurer, P. Lindner, S. Förster, Colloidal quasicrystals with 12-fold and 18-fold diffraction symmetry, Proc. Natl. Acad. Sci. 108 (2011) 1810. [2] A. Exner, S. Rosenfeldt, S. Fischer, P. Lindner, S. Förster, Defect accommodation in nanostructured soft crystals, Nanoscale 2013, in press

CPP 9.2 Mon 15:30 ZEU 260

The Flexible Rare Event Sampling Harness System (FRESHS) — KAI KRATZER¹, JOSHUA BERRYMAN², AARON TAUDT¹, JOHANNES ZEMAN¹, and ●AXEL ARNOLD¹ — ¹Institut für Computerphysik, Universität Stuttgart, Germany — ²Theory of Soft Condensed Matter, University of Luxembourg, Luxembourg

Nucleation is a rare event that is computationally expensive to study in brute force computer simulations. Special sampling techniques can reduce this effort. We present the Flexible Rare Event Sampling Harness System (FRESHS), an open source software framework (<http://www.freshs.org>) that provides Forward Flux Sampling (FFS) and Stochastic Process Rare Event Sampling (S-PRES), which are two such methods well suited to study nucleation events.

Several features of FRESHS make its application particularly easy. FFS or S-PRES only require an order parameter that describes the progress of the rare event and allows to split the transition into milestones or interfaces. Our FFS implementation features automatic interface placement, which ensures optimal flux through all interfaces without the need of expert knowledge. ‘Ghost’ runs overcome the computational bottleneck of waiting for the last trial simulation when advancing to the next interface. FRESHS can steer popular Molecular Dynamics codes such as GROMACS, LAMMPS or ESPResSo, and other software can be attached through a simple plugin system. Our framework allows for checkpointing and flexible analysis already during runtime, and is suitable for single workstations up to large compute clusters.

CPP 9.3 Mon 15:45 ZEU 260

Modelling the structure of tubular J-aggregates using MD-simulations and MD-based calculations of exciton spectra —

●JÖRG MEGOW¹, STEFAN KIRSTEIN¹, MERLE RÖHR², MARCEL SCHMIDT AM BUSCH³, ROLAND MITRIĆ², THOMAS RENGER³, JÜRGEN P. RABE¹, and VOLKHARD MAY¹ — ¹Humboldt-Universität zu Berlin, Deutschland — ²Julius-Maximilians-Universität, Würzburg, Deutschland — ³Johannes Kepler Universität, Linz, Österreich

Tubular J-aggregates composed of amphiphilic cyanine dyes have been studied in [1,2]. Two different approaches were used to build a molecular model of the structure: First, a theoretical model based on absorption spectra and on orientations of transition dipoles was translated into real arrangements of molecules [1]. Second, molecules were packed to reproduce best a structure model based on high resolution cryo-TEM [2]. For the first time now, molecular dynamics (MD) simulations of the aggregates in solution together with MD-based calculations of optical spectra are utilized to study the structure of the system. MD simulations of both structure models show that the model of [1] is unstable, while the model that is consistent with [2] is stable during MD simulation. Based on the simulations, Frenkel exciton spectra for both structure models have been computed. It will be shown that a detailed calculation of the energy transfer coupling, including screening effects, allows for a reasonably good description of the absorption spectrum also for the second structure model.

[1] D. Eisele, et al., Nature Chemistry 4, 655-662 (2012)

[2] H. v. Berlepsch et al., Chem. Phys. 285, 27-34 (2011)

CPP 9.4 Mon 16:00 ZEU 260

Relaxation of the complex heat capacity of eicosane in the metastable rotator phase. — ●CARLO DI GIAMBATTISTA, JÖRG BALLER, and ROLAND SANCTUARY — Laboratory for the Physics of Advanced Materials, University of Luxembourg

Some normal alkanes show stable and/or meta-stable polymorphisms. Understanding the process behind the formation of these structures for n-alkanes ($n \geq 20$) could yield a better understanding of the crystallisation of polymers [1]. Upon cooling from the melt eicosane ($C_{20}H_{42}$) exhibits a transition to a metastable orthorhombic phase (rotator I) [2]. Upon further cooling there is a second transition to a stable triclinic structure. In this work, we investigate the metastable phase with Temperature Modulate Differential Calorimetry (TMDSC). We use stochastic temperature perturbations (TOPEM[®]-Mettler Toledo). This allows us to get a frequency dependant complex heat capacity $c_p^*(\omega)$. In the metastable rotator phase the heat capacity of eicosane becomes time dependant. In the frequency domain its complex heat capacity can be described by a temperature dependant Debye relaxator. There are two distinct temperature regions, one in which the relaxation time diverges on approaching the melting temperature and another region with an almost constant relaxation time at lower temperatures.

[1] Ungar, G. and N. Masic (1985). J. Phys. Chem. 89(6): 1036-1042.

[2] Sirota, E. B., H. E. King, et al. (1993). J. of Chem. Phys. 98(7): 5809-5824.

CPP 9.5 Mon 16:15 ZEU 260

Crystallization of Charged Macromolecules using FRESHS — ●KAI KRATZER and AXEL ARNOLD — Institute for Computational Physics, University of Stuttgart, Allmandring 3, 70569 Stuttgart, DE
The investigation of nucleation, e.g. the onset of crystal growth, of proteins or colloids is demanding both in experiments and computer simulations because nucleation is a rare event. Such an event will simply not happen in the limited system sizes that can be observed experimentally or in brute force computer simulations, in particular close to the coexistence line where the energy barrier is high. However, in computer simulations this can be overcome by special simulation techniques such as Forward Flux Sampling (FFS).

Combining our parallel molecular dynamics code ESPResSo and our FFS framework FRESHS, the Flexible Rare Event Sampling Harness System, we performed computer simulations of the fluid-solid nucleation close to the coexistence line of Yukawa particles, a simple model for charged colloids. We observe a two stage nucleation process with a metastable structure forming first for a broad range of parameters and we compare to the expectations of the Classical Nucleation Theory.

15 min break

CPP 9.6 Mon 16:45 ZEU 260

Stability of crystal nuclei in poly(ϵ -caprolactone), studied by fast scanning calorimetry — ●EVGENY ZHURAVLEV, ANDREAS WURM, JÜRN SCHMELZER, and CHRISTOPH SCHICK — Universität Rostock, Institut für Physik, Rostock, Germany

Thermal stability of crystal nuclei was tested in poly(ϵ -caprolactone) at increasing temperatures. The DFSC allows controlled fast heating and cooling of the sample and determination of its heat capacity at scanning rates up to 100,000 K/s. The possibility to change the temperature so rapidly that there is no time for significant recrystallization of the crystals (or nuclei), allows successive isothermal studies of melting, reorganization and recrystallization. Comparison of isothermal crystallization with and without pretreatment at lower temperatures can be realized. The key question we are trying to answer is up to what temperature the various structures can influence on a successive crystallization after disordering. The structures range from configurations having practically unmeasurable latent heats of disordering (melting) to being clearly-recognizable, ordered species with rather sharp disordering endotherms in the temperature range from the glass transition to equilibrium melting for increasingly perfect and larger crystals. Preliminary experiments show, that the PCL nuclei, formed at 210 K (homogeneous nucleation) significantly speeds up crystallization at 250 K, but do not exist anymore at 300 K ($T_m = 343$ K).

CPP 9.7 Mon 17:00 ZEU 260

In-situ crystal thickening in semi-crystalline diblock copolymer under soft confinement — ●ROBERT SCHULZE¹, STEFAN HÖLZER², and KLAUS JANDT¹ — ¹Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Löbdergraben 32, 07743 Jena, Germany — ²Laboratory of Organic Chemistry and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstraße 10, 07743 Jena, Germany

Crystal thickening of soft-confined semi-crystalline diblock copolymers requires a rearrangement of the microdomain structure.

In the current study the crystal thickening and microdomain rearrangement of a polybutadiene-block-poly(ethylene oxide) was investigated in-situ in the bulk and on the surface of thin films by X-ray scattering and in-situ atomic force microscopy, respectively.

Initially, crystallized bulk and thin film samples were annealed at selected temperatures determined by differential scanning calorimetry. In the bulk we found a sigmoidal increase of the lamellar long period during annealing. On the thin film surface we observed that the formation of thicker lamellae results from a complex interaction between the melting of some crystalline microdomains and the thickening of the adjacent ones. Further we discovered the growth of crystalline double lamellae that consisted of non-interdigitated extended chains.

The mechanism of crystal thickening can be used to fabricate tunable nanopatterns of amphiphilic semi-crystalline diblock copolymers which are interesting e.g., in the photonics or the biomedical field.

CPP 9.8 Mon 17:15 ZEU 260

Pattern Formation in Polymer Single Crystals — HUI ZHANG¹, BIN ZHANG¹, MAXIMILIAN VIELHAUER², ROLF MÜLHAUPT^{2,3}, MORITZ BAIER⁴, STEFAN MECKING⁴, and ●GÜNTER REITER^{1,3} — ¹Institute of Physics, University of Freiburg, 79104 Freiburg, Germany — ²Institut für Makromolekulare Chemie, University of Freiburg, 79104 Freiburg, Germany — ³Freiburger Materialforschungszentrum, University of Freiburg, 79104 Freiburg, Germany — ⁴Department of Chemistry, University of Konstanz, 78464 Konstanz, Germany

Polymer crystals typically grow at conditions far from thermodynamic equilibrium, resulting in chain-folded lamellar crystals. Even in single crystals, characterized by dendritic or faceted structures with a well-defined envelope reflecting the underlying crystal unit cell, polymers are folded and thus in a meta-stable state. Systematic investigations on such crystals led to a general concept of a nucleation of secondary lamellar crystals induced by an insertion mechanism on the amorphous fold surfaces. These secondary lamellar crystals are in registry with the underlying single crystal. The dependence of the number density of secondary lamellae on the width of the side branches of the underlying crystal suggests that nucleation was controlled by the morphology of the underlying crystal which, in turn, could be tuned by crystallization temperature and film thickness. Moreover, annealing such meta-stable single crystals allowed to unveil the initial morphological framework of a dendritic single crystal, i.e. the initial stages of growth.

CPP 9.9 Mon 17:30 ZEU 260

Tailoring diblock copolymer surface nanostructures by crystal thickening — ●ROBERT SCHULZE, MATTHIAS ARRAS, and KLAUS JANDT — Otto Schott Institute of Materials Research (OSIM), Friedrich Schiller University Jena, Löbdergraben 32, 07743 Jena, Germany

One approach to control the thickness of crystalline lamellae in the bulk is the self-nucleation experiment. But crystal thickening might be useful to tailor surface nanostructures of semi-crystalline copolymer thin films.

In this present study of a polybutadiene-block-poly(ethylene oxide), we correlate within two self-nucleation experiments, i.e., in the bulk and thin film, the calorimetric bulk properties to the resulting thin film surface nanostructures which enables the prediction of the surface nanostructure formation.

In a self-nucleation experiment, crystalline standard samples were annealed at temperatures in the melting range. Low temperature annealing promoted the thickening of crystalline lamellae on the film surface which is explained by the formation of less folded chain crystals that exhibit increased melting temperatures. Based on a theoretical analysis, we identified a functional dependence of calorimetric bulk properties on lamellar thickness which can be used to predict the lamellae thickness as a function of the annealing temperature.

We established the dual self-nucleation experiment as a powerful tool to predictably tailor surface nanostructures in the range of several nanometers.

CPP 9.10 Mon 17:45 ZEU 260

Evolution of Entanglement Distribution in the Growth and Melting of a Polymer Single Crystal — ●CHUANFU LUO¹ and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden, Germany — ²Technische Universität Dresden, Germany

Many physical properties of polymers are determined by the state of entanglement, such as visco-elasticity. Another closely related topic is the crystallization and melting of polymers, in which the formation of folded chain segments are strongly related with the local entanglement states [1]. Computer simulation provides the possibility to study the changes in entanglement states during the phase transition of polymers. We developed a method to calculate the local entanglement length based on an extended primitive path analysis (PPA) [2]. We apply this method to calculate the evolution of entanglement distribution in the growth and melting of a polymer single crystal, which are achieved by large scale MD simulations. In principal, the method can be used to calculate the entanglement distribution in various conditions, such as with confinement and during dynamic processes.

[1]C. Luo and J.-U. Sommer, ACS Macro Lett. 2, 31(2013)

[2]R. Everaers et al., Science 303, 823-826 (2004)

CPP 10: Wetting, Micro and Nanofluidics

Time: Monday 15:00–16:15

Location: ZEU 114

CPP 10.1 Mon 15:00 ZEU 114

Capillary focusing: New Breakup Regimes in Step-Emulsification — ●MICHAEL HEIN¹, SHAHRIAR AFKHAM², LOU KONDIC², and RALF SEEMANN¹ — ¹Experimental Physics, Saarland University — ²Department of Mathematical Sciences, New Jersey Institute of Technology

Droplet based microfluidics has become very popular, both in research and application. But despite of a large number of studies on the droplet breakup, the physics behind this mechanism is only poorly understood. We present experimental research on the formation of droplets in a particular step-geometry by the breakup of a liquid filament. This non-equilibrium process arises from the interplay between flow properties and interfacial instabilities when the filament is suddenly released from a quasi 2d confinement at a topographic step. In particular we investigate the transition between two breakup mechanisms: the 'step-regime' where small droplets are generated just at the step and the 'jet-regime', where larger droplets are formed at some distance after the step. We provide experimental evidence that the breakup mechanism can be controlled by tuning the Capillary number and the channel geometry, which is supported by numerical simulations using the volume-of-fluid method. Interestingly, we observe new breakup mechanisms appearing during the transition from the 'step-' to the 'jet-regime' for large aspect ratios of the liquid filament.

CPP 10.2 Mon 15:15 ZEU 114

Layer erosion by crossflow: in-situ detection using microfluidics and GISAXS — GERD HERZOG¹, MATTHIAS SCHWARTZKOPF¹, BERIT HEIDMANN¹, SHUN YU¹, FRANS DE JONG², MICHAEL SCHLÜTER², VOLKER KÖRSTGENS³, PETER MÜLLER-BUSCHBAUM³, and ●STEPHAN V. ROTH¹ — ¹DESY, Notkestr. 85, D-22607 Hamburg, Germany — ²Institute of Multiphase Flows, Hamburg University of Technology, Eißendorfer Str. 38, D-21073 Hamburg, Germany — ³TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, D-85748 Garching, Germany

The process of inorganic coating (scaling) and fouling of organic matter under crossflow conditions is very important in many technical applications, e.g. membrane modules, heat exchangers, coatings for surfaces (airplanes, automobiles, ships), windows, textiles, etc. Despite this fact, the physical process of scaling and fouling as well as the reduction of scaling and fouling under crossflow conditions is not well understood because the molecular interaction forces between particles and surface are difficult to estimate and the shear stresses that act at the particles are difficult to describe. Therefore we use microbeam grazing incidence small-angle X-ray scattering (μ GISAXS) to investigate the dynamic deposition and erosion behavior of particles at surfaces. Polymeric colloids on a glass plate have been detected in a microfluidic cell by means of μ GISAXS under water crossflow conditions. Depending on the choice of colloidal layer (surface functionalization), the time series of the measurements show a significant reduction of colloids on the surface and thereby image the erosion process quantitatively.

CPP 10.3 Mon 15:30 ZEU 114

Relaxation and Intermediate Asymptotics of a Surface Perturbation in a Viscous Film — ●OLIVER BÄUMCHEN¹, MICHAEL BENZAQUEN², THOMAS SALEZ², JOSHUA D. MCGRAW³, MATILDA BACKHOLM⁴, PAUL FOWLER⁴, ELIE RAPHAËL², and KARI DALNOKI-VERESS⁴ — ¹Max Planck Institute for Dynamics & Self-Organization, 37077 Göttingen, Germany — ²Laboratoire de Physico-Chimie Théorique, UMR CNRS Gulliver 7083, ESPCI, Paris, France — ³Department of Experimental Physics, Saarland University, 66123 Saarbrücken, Germany — ⁴Department of Physics and Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, Canada

The surface of a thin liquid film with non-constant curvature flattens as a result of capillary forces. While this levelling process is driven by local curvature gradients, the global boundary conditions greatly influence the dynamics. Here, we study the evolution of re-entrant trenches in a polystyrene nanofilm. We report on full agreement between theory and experiments for the capillary-driven flow and resulting time dependent height profiles, a crossover in the power law dependence of the viscous energy dissipation as a function of time as the trench evolution transitions from two noninteracting to interacting steps, and the convergence of the profiles to a universal self-similar attractor that is given by the Green's function of the linear operator describing the dimensionless linearized thin film equation.

O. Bäumchen et al., *Phys. Rev. E* **88**, 035001 (2013).

CPP 10.4 Mon 15:45 ZEU 114

The Rayleigh-Plateau Instability on a Fiber Revisited - Influence of the Hydrodynamic Boundary Condition — ●SABRINA HAEFNER^{1,4}, OLIVER BÄUMCHEN^{2,4}, MICHAEL BENZAQUEN³, THOMAS SALEZ³, ROBERT PETERS⁴, JOSHUA MCGRAW¹, ELIE RAPHAËL³, KARIN JACOBS¹, and KARI DALNOKI-VERESS^{3,4} — ¹Saarland University, Experimental Physics, 66041 Saarbrücken, Germany — ²Max Planck Institute for Dynamics & Self-Organization, 37077 Göttingen, Germany — ³Laboratoire de Physico-Chimie Théorique, UMR CNRS Gulliver 7083, ESPCI, Paris, France — ⁴McMaster University, Department of Physics and Astronomy, Hamilton L8S4M1, Canada

The Rayleigh-Plateau Instability (RPI) of a liquid column underlies a variety of hydrodynamic phenomena that can be observed in everyday life. In the classical case of a free liquid column, linear perturbation theory predicts characteristic rise-times and wavelengths. However, the description of a liquid layer on a fiber requires the consideration of the solid/liquid interface in addition to the free interface. In this study, we revisit the RPI of a viscous liquid layer on a solid fiber by varying the hydrodynamic boundary condition at the fiber/liquid interface. The rise of the amplitudes of the surface undulations is precisely tracked and the growth rate of the instability is determined for the different slip boundary conditions and compared to the theoretical models.

CPP 10.5 Mon 16:00 ZEU 114

Following structural changes in nanoparticle films under laminar flow conditions with in-situ SAXS microfluidics — ●VOLKER KÖRSTGENS¹, MARTINE PHILIPP¹, DAVID MAGERL¹, MARTIN A. NIEDERMEIER¹, JOHANNES SCHLIPP¹, LIN SONG¹, GONZALO SANTORO², VASYL HARAMUS³, STEPHAN V. ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — ²DESY, Notkestr. 85, 22603 Hamburg — ³Helmholtz-Zentrum Geesthacht: Zentrum für Material- und Küstenforschung GmbH, 21502 Geesthacht

Microfluidic processes which are accompanied with structural changes at the solid-liquid interface are monitored with in-situ small angle x-ray scattering (SAXS) using a micro-focused x-ray beam. Changes of the nanostructure of a film of nanospheres dispersed in a matrix of sodium alginate of algal origin and its cross-linked analogue are followed during flow of water through a microfluidic channel. The study includes the investigation in transmission through the channel walls (SAXS) as well as in grazing incidence addressing the nanoparticle films on the substrate (GISAXS). Structural changes caused by the laminar flow in the microfluidic channel are traced and demonstrate the possibilities of both complementary in-situ SAXS techniques.

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

CPP 11: Interfaces and Thin Films I

Time: Monday 16:30–18:30

Location: ZEU 114

CPP 11.1 Mon 16:30 ZEU 114

Guiding Reorganization in Block Copolymer Thin Films on the Nanoscale by Judicious Control of Solvent Vapor Exposure — ALESSANDRO SEPE¹, DORTHE POSSELT², JIANQI ZHANG¹, JAN PERLICH³, DETLEF-M. SMILGIES⁴, ANDREY A. RUDOV⁵, IGOR I. POTECHKIN⁵, and CHRISTINE M. PAPADAKIS¹ — ¹TU München, Garching — ²Roskilde University, Denmark — ³DESY, Hamburg — ⁴Cornell University, Ithaca, NY, USA — ⁵Lomonosov Moscow State University, Russian Federation

A perfect alignment of nanostructured block copolymer thin films is mandatory for their applications. Solvent vapor annealing is a method to improve order in films prepared by spin-coating. We investigate thin films of lamellar poly(styrene-*b*-butadiene) (P(S-*b*-B)) in cyclohexane vapor. The rates of swelling in solvent vapor and drying as well as the maximum degree of swelling of the film are controlled. The structural changes are monitored in-situ using time-resolved grazing-incidence small-angle X-ray scattering (GISAXS). Good alignment of the lamellar nanostructure is achieved for a sufficiently high degree of swelling and is even further improved during drying, provided the rate of drying is sufficiently low. A second swelling/drying cycle shows that equilibrium has been achieved. During swelling, the lamellar stack rearranges as soon as T_g of PS is crossed, and additional lamellae are formed. During (slow) drying, this new structure is conserved. Computer simulations confirm this mechanism [2].

1. A. Sepe et al., submitted.

2. A.A. Rudov et al., *Macromolecules* **46**, 5786 (2013)

CPP 11.2 Mon 16:45 ZEU 114

Diblock-copolymer thin films under shear — LENIN S. SHAGOLSEM^{1,2}, TORSTEN KREER¹, and JENS-UWE SOMMER^{1,2} — ¹Leibniz Institute of Polymer Research Dresden — ²TU Dresden

By employing molecular dynamics simulations we study the behavior of copolymer thin films under shear. In particular, we consider symmetric diblock-copolymer melts confined by two non-selective walls. Since there is no preferential interaction between the walls and the components of the diblock-copolymer a vertically oriented lamellar structure is formed. We investigate the response of the system to transverse and perpendicular modes of shear and study shear deformation of the lamellae, reorientation transition in transverse shear, and flow behavior. We find that the inclined lamellae state (observed for transverse shear below a critical shear rate) is stabilized by a cyclic motion of chains. Above a critical shear rate, the lamellae orient along the direction of flow. Furthermore, the macroscopic response is investigated by kinetic friction coefficient and shear viscosity. We observe that the critical shear rate, at which the lamellae reorientation occurs, coincides with the onset of shear-thinning.

CPP 11.3 Mon 17:00 ZEU 114

Structural evolution of perpendicular lamellae in diblock copolymer thin films during solvent vapor treatment investigated by GISAXS — JIANQI ZHANG¹, DORTHE POSSELT², ALESSANDRO SEPE¹, XUHU SHEN¹, JAN PERLICH³, DETLEF-M. SMILGIES⁴, and CHRISTINE M. PAPADAKIS¹ — ¹TU München, Physik-Department, Garching — ²IMFUFU, Roskilde University, Denmark — ³DESY, Hamburg — ⁴Cornell University, Ithaca, NY, USA

Drastic structural rearrangements in block copolymer thin films occur during solvent vapor treatment. Their understanding is mandatory for the use of solvent vapor treatment for annealing defects otherwise hampering applications. We investigate the structural evolution in poly(styrene-*b*-butadiene) (P(S-*b*-B)) diblock copolymer thin films featuring perpendicular lamellae. The changes during solvent vapor treatment are studied in-situ using time-resolved grazing-incidence small-angle X-ray scattering (GISAXS) [1]. The swelling of the film is one-dimensional along the substrate normal. During swelling, the initially perpendicular lamellae tilt within the film to be able to shrink, as confirmed by computer simulations [2]. In contrast, at the film surface, the lamellae stay perpendicular, and eventually vanish at the expense of a thin PB wetting layer. During the subsequent drying, the perpendicular lamellae reappear at the surface, and finally, PS blocks protrude. By modeling, the time-dependent height of the protrusions can be quantitatively extracted.

1. J. Zhang et al., *Macromol. Rapid Commun.* **34**, 1289 (2013)2. A.A. Rudov et al., *Macromolecules* **46**, 5786 (2013)

CPP 11.4 Mon 17:15 ZEU 114

Highly enhanced ordering dynamics in solvent-annealed block-copolymer films supported by a polymer network — ANJA STENBOCK-FERMOR¹, LARISA TSARKOVA¹, ALEXANDER BÖKER¹, and ARMIN KNOLL² — ¹DWI at RWTH-Aachen University, Forckenbeckstraße 50, 52074 Aachen — ²IBM Research GmbH, Säumerstrasse 4, CH-8803 Rüschlikon Switzerland

We studied the solvent driven ordering dynamics of block copolymer films supported by a densely cross-linked organic hard mask (HM) designed for lithographic fabrication. We found that the ordering of microphase separated domains on the HM layer proceeds significantly faster as compared to similar films on silicon wafers. Both the dynamics of terrace-formation as well as the long-range lateral ordering of the microdomains is greatly enhanced. The effect is independent on the chemical structure and volume composition (cylinder-/ lamella-forming) of the studied block copolymers. Importantly, enhanced ordering is achieved even at a reduced degree of swelling corresponding to an intermediate to strong segregation regime, when similar films on conventional substrate show very limited ordering. In-situ ellipsometric measurements of the swollen films revealed an insignificant increase by 1-3 vol. % in the solvent up-take by HM-supported films. Therefore we attribute the enhanced dynamics to reduced interactions at the block copolymer/HM-support interface. Apart from immediate technological impact in block copolymer-assisted nanolithography, our findings convey novel insight into effects of molecular architecture on polymer-solvent interactions.

CPP 11.5 Mon 17:30 ZEU 114

Tuning the Monolayer Properties of Liquid Crystalline Septithiophenes — KHOSROW RAHIMI¹, WIM DE JEU¹, ULRICH ZIENER², MARTIN MÖLLER¹, and AHMED MOURRAN¹ — ¹DWI Interactive Materials Research at RWTH Aachen, Germany — ²Institute of Organic Chemistry III, University of Ulm, Albert-Einstein-Allee 11, 89081 Ulm, Germany

Conjugated molecules including oligothiophenes are promising materials for organic electronic devices due to the combination of low-cost solution processing and charge transport mobility. The conduction in thin polycrystalline films is limited by the degree of crystallinity and the extent of the crystalline domains. To optimize single crystal devices in monolayers, crystal growth involves the delicate point of decoupling of lateral (two-dimensional) growth from that perpendicular to the substrate. The growth kinetics of molecular thin films will be influenced by possible liquid crystal (LC) order due to anisotropy in molecular structure. New terminally substituted oligothiophenes have been synthesized, that exhibit thermotropic LC phases. They consist of a conjugated thiophene backbone to which long flexible alkyl chains are attached that incorporate a bulky -Si(CH₃)- group. Varying the position of -Si(CH₃)- in the linear alkyl chain, we find that the temperature window of LC phase is larger when -Si(CH₃)- is situated away from the thiophene core. As a result the monodomain size is enhanced. However, this trend is vice versa when the Si group is very close to the core. We conclude that deposition and formation of monolayer and its monodomain size is controlled with LC phase.

CPP 11.6 Mon 17:45 ZEU 114

FTIR Imaging of PFSA Membranes for Fuel Cells — PAWEŁ GAZDZICKI¹ and MARTINA CORASANITI² — ¹German Aerospace Center (DLR), Institute of Technical Thermodynamics, Pfaffenwaldring 38-40, 70569 Stuttgart, Germany — ²Solvay Specialty Polymers, viale Lombardia 20, 20021 Bollate (MI), Italy

In our presentation we provide an attenuated total reflection (ATR) Fourier transform infrared (FTIR) imaging study of perfluorosulfonic acid (PFSA) membranes. These materials are typically used as ion conductors in electrochemical energy converters such as low temperature fuel cells. The spectroscopic images have been measured using a focal plane array detector allowing for a lateral resolution of 1 μ m. Thanks to this superior resolution it is possible to detect statistically distributed areas with increased hydrophobicity which exhibit a reduced concentrations of sulfonic acid groups and an increased concentration of the polytetrafluoroethylene (PTFE) backbone. For

Aquivion® the diameter of the individual regions of $-\text{SO}_3^-$ depletion is found to be 5 - 15 μm ; the overall percentage of area with reduced SO_3^- occurrence is about 1.5 - 2% of the analysed surface area. Additionally, we compare FTIR transmission and ATR spectra that provide bulk and surface specific information, respectively.

The research leading to these results has received funding from the European Union's Seventh Framework Programme (FP7/2007-2013) for Fuel Cell and Hydrogen Joint Technology Initiative under Grant No. 303452 (Impact).

CPP 11.7 Mon 18:00 ZEU 114

Gas permeation of carbon nanomembranes — •VAHE CHINARYAN¹, MIN AI¹, SERGEY SHISHATSKIY², JAN WIND², XIANGHUI ZHANG¹, CHRISTOPH T. NOTTBOHM¹, NILS MELLECH¹, ANDREAS WINTER¹, HENNING VIEKER¹, JUN QIU³, KARL-JOSEF DIETZ⁴, ARMIN GÖLZHÄUSER¹, and ANDRE BEYER¹ — ¹Physics of Supramolecular Systems, University of Bielefeld, 33615 Bielefeld, Germany — ²Institute of Polymer Research, Helmholtz-Zentrum Geesthacht, 21502 Geesthacht, Germany — ³Performance Materials-Chemistry & Technology, DSM, 6160 MD Geleen, The Netherlands — ⁴Plant Biochemistry and Physiology, University of Bielefeld, 33615 Bielefeld, Germany

Gas permeation characteristics of carbon nanomembranes (CNMs) from self-assembled monolayers are reported for the first time. The assembly of CNMs onto polydimethylsiloxane (PDMS) support membranes allows determination of gas permeation characteristics. Single layer and triple layer CNMs with thicknesses of 1 nm and 3 nm were investigated in respect to permeation of hydrogen, helium, carbon dioxide, oxygen, nitrogen, argon, methane and ethane. In addition,

the CNM-PDMS composites were characterized by X-ray photoelectron spectroscopy, helium-ion microscopy as well as atomic force microscopy. A careful analysis about the contribution of the PDMS support membranes to the gas permeation allowed an estimate of the intrinsic CNM permeances. These values indicate a molecular sieve-like property of CNMs which is attributed to molecular-sized channels in CNMs.

CPP 11.8 Mon 18:15 ZEU 114

Perfluorinated compound rigidifies model lipid membrane — •BEATE-ANNETTE BRÜNING¹ and BELA FARAGO² — ¹Soft Matter and Functional Materials, Helmholtz Zentrum Berlin, Berlin, Germany — ²Time-of-Flight and High Resolution, Institut Laue-Langevin, Grenoble, France

We report a combined dynamic light scattering (DLS) and neutron spin-echo (NSE) study on vesicles composed of the phospholipid 1,2-dimyristoyl-sn-glycero-3-phosphatidylcholine (DMPC) under the influence of varying amounts of perfluorooctanoic acid (PFOA). Mechanical properties of a model membrane and the corresponding bilayer undulation dynamics can be specifically influenced by changing its composition. We have performed DLS on vesicles composed of DMPC/PFOA mixtures to investigate changes in their respective size and corresponding center-of-mass diffusion. We study bilayer undulation and bulk diffusion dynamics using NSE, on time scales up to 200 ns. We calculate the bilayer bending rigidities κ for varying ratios of the perfluorinated compound, and obtain a bilayer stiffening for increasing amounts of the perfluorinated surfactant. Similar to the effect evoked by cholesterol, we attribute the observed stiffening to a condensing effect of the perfluorinated compound on the lipid bilayer.

CPP 12: Focus Session: Feedback Control of Nonlinear Soft and Hard Matter Systems (original: DY, joined by CPP)

Feedback control methods, which are well established in the field of nonlinear sciences, have recently entered new areas such as pattern formation in non-equilibrium soft-matter systems, Brownian transport and quantum transport. The focus session provides a platform for the presentation and discussion of state-of-the-art results and for pointing out open problems in this emerging field. (Organizers S. Klapp and E. Schöll)

Time: Monday 15:00–17:45

Location: HÜL 186

Invited Talk CPP 12.1 Mon 15:00 HÜL 186
Feedback and information processing in stochastic thermodynamics — •UDO SEIFERT — II. Inst. für Theoretische Physik, Universität Stuttgart

Stochastic thermodynamics provides a framework for describing feedback control of colloidal and molecular systems [1]. A crucial concept is the notion of optimal finite-time protocols that transform a given initial distribution to a given final one in finite time with minimal thermodynamic cost [2]. If additional information becomes available through a measurement of the state of the system, one can thus even extract work from a single heat bath [3]. Fluctuation theorems taking into account this concept of information lead to bounds on the efficiency of such Brownian information machines [4]. These feedback-based schemes will be compared to autonomous information processing as it occurs in cellular sensing [5].

- [1] U Seifert, Rep. Prog. Phys. 75, 126001, 2012
- [2] T Schmiedl and U Seifert, Phys. Rev. Lett. 98, 108301, 2007
- [3] M Bauer, D Abreu, and U Seifert, J. Phys. A 45, 162001, 2012
- [4] D Abreu and U Seifert, Phys. Rev. Lett. 108, 030601, 2012
- [5] AC Barato, D Hartich, and US, Phys. Rev. E 87, 042104, 2013

Invited Talk CPP 12.2 Mon 15:30 HÜL 186
Thermophoretic trapping and steering of single nano-objects with plasmonic nanostructures — •FRANK CICHOS¹, ANDREAS BREGULLA¹, MARCO BRAUN¹, and HAW YANG² — ¹Molecular Nanophotonics Group, Institute of Experimental Physics I, University Leipzig, 04103 Leipzig, GERMANY — ²Department of Chemistry, Princeton University, Princeton, NJ 08544-2020, USA

The manipulation of single micro- and nano-particles or even single molecules in solution requires to beat Brownian motion with a mechanism that drives objects into a well defined direction. Such a mechanism is provided by the thermophoretic drift of nano-objects in a tem-

perature gradient as generated by optically heated plasmonic nanostructures. Since these tiny heat sources can be switched optically at high frequencies, they provide new means of feedback controlled optical manipulations. Here we report on two experiments controlling individual particles in solution by such a feedback mechanism. The first experiment employs a self-propelled thermophoretic swimmer that is steered in solution by a real-time feedback of the swimmer orientation and position. This type of feedback controlled actuation predicts an increased positional control with decreasing particle size. The second experiment involves the trapping of single colloids and molecules in feedback controlled dynamic temperature fields. While the actual thermophoretic drift is repelling the object from the heat source, the dynamic switching provides an effective potential well, which can be shaped by the feedback details. Both experiments provide huge perspectives for study of interactions in well defined clusters of nano-objects.

CPP 12.3 Mon 16:00 HÜL 186

Manipulating rheology of colloidal particles at surfaces — •TARLAN A. VEZIROV, SASCHA GERLOFF, and SABINE H. L. KLAPP — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

Colloidal particles under the combined influence of an external driving force and restricted geometry exhibit a wealth of non-linear phenomena, which are relevant in diverse fields such as directed particle transport, sorting mechanisms and friction phenomena at the nanoscale. We perform computer simulations of a confined bilayer system of charged colloidal particles interacting via a combined softsphere- and Yukawa-potential. The model parameters are adjusted according to ludox silica particles, which we have previously studied under equilibrium conditions [1]. As a framework for solving the equation of motion, we employ overdamped Brownian dynamics simulations. Switching on an exter-

nal shear flow we find, a sequence of states characterised by pinning, shear-induced melting and reentrant ordering into a moving hexagonal state with synchronised oscillations of the particles [1]. By adding an additional feedback equation of motion we are able to stabilise specific properties such as the degree of hexagonal ordering or the shear stress. This opens the route for a deliberate control of friction properties.

[1] S. Grandner and S.H.L. Klapp, *J. Chem. Phys.* **129**, 244703 (2008).

[2] T. A. Vezirov and S. H. L. Klapp, *Phys. Rev. E* **88**, 5 (2013).

CPP 12.4 Mon 16:15 HÜL 186

Optimal control of particle separation in inertial microfluidics — ●CHRISTOPHER PROHM and HOLGER STARK — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin

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 investigate the motion of a colloidal particle in microfluidic channels using mesoscopic simulations [3]. We show how the geometry of the channel influences inertial focussing. We also demonstrate that manipulating the axial or angular velocity of the particle modifies the inertial lift force profile which permits control of the lateral particle position. Finally we apply the theory of optimal control to the problem of particle sorting in inertial microfluidics [4]. We design optimal force profiles that are able to steer particles to desired lateral positions and, most importantly, to separate particles of similar size in a very robust fashion.

[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] C. Prohm, F. Tröltzsch, and H. Stark *EPJE*, **36**, 118 (2013).

15 min. break

CPP 12.5 Mon 16:45 HÜL 186

Time-delayed feedback control of the Dicke-Hepp-Lieb superradiant quantum phase transition — ●WASSILI KOPYLOV¹, CLIVE EMARY², ECKEHARD SCHÖLL¹, and TOBIAS BRANDES¹ — ¹Institut für

Theoretische Physik, Technische Universität Berlin — ²Department of Physics and Mathematics, University of Hull, United Kingdom

We apply the time-delayed Pyragas control scheme to the dissipative Dicke system, modulating it by the difference of photon numbers emitted from the cavity. Using the mean field approach and linear stability analysis we show that this control dramatically affects the states in the primary superradiant regime, creating new limit cycle phases and a rich phase diagram. We also derive an analytical transcendental equation for the boundaries between the different zones in the phase diagram.

CPP 12.6 Mon 17:00 HÜL 186

Time-delayed control of (un)stable steady states in open quantum systems — ●PHILIPP STRASBERG and TOBIAS BRANDES — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin, Germany

We consider the quantum version of classical time-delayed feedback to control (un)stable steady states of a quantum system. The system is then described by a (non-linear) stochastic master equation, which can be mapped to a set of time-delayed stochastic differential equations for the means and a set of a non-linear equations for the covariances. At steady state, the equations for the means are on average the same as for the classical case with a stochastic part coming purely from the quantum measurement and feedback.

Invited Talk

CPP 12.7 Mon 17:15 HÜL 186

Feedback control in quantum transport — ●CLIVE EMARY — Department of Physics and Mathematics, University of Hull, United Kingdom

Quantum transport is the study of the movement of electrons in structures small enough that the quantum properties of the electron play an important role. Recent “full counting statistics” experiments provide detailed time-resolved information on the stochastic motion of electrons in such structures which, it is proposed, could form the basis of feedback control schemes for quantum transport. Such feedback control has been shown to give rise to many interesting effects such as the suppression of unwanted current fluctuations, the realisation of a nanoelectric Maxwell’s daemon and the stabilisation of non-equilibrium pure states.

In this talk I will review these proposals and discuss the effects of delay on such quantum feedback schemes. I will conclude with some perspectives on the use of coherent — as opposed to measurement-based — quantum control strategies in the transport setting.

CPP 13: Glasses (original: DY, joined by DF, CPP)

Time: Monday 15:00–17:30

Location: ZEU 146

CPP 13.1 Mon 15:00 ZEU 146

Dynamic Crossover and Stepwise Solidification of Confined Water — ●MATTHIAS SATTIG and MICHAEL VOGEL — Hochschulstraße 6, D-64289 Darmstadt

The dynamical behaviour of water in the regime of the supercooled liquid is still a topic of large interest. In particular, the existence of a fragile-to-strong transition (FST) at around 225K induced by a liquid-liquid phase transition (LL) is controversially discussed [1]. The proposed temperature range of the FST is hardly accessible in bulk water.

Our ²H NMR investigation reveals two dynamic crossovers of supercooled water in nanoscopic (nm) confinement. A dynamic crossover of liquid water at ca. 225K is accompanied by a formation of a fraction of solid water. Therefore, this effect can not be attributed to the LL, but rather to a change from liquid-like to interface-dominated dynamics. Moreover, the ²H NMR data yield evidence that the α process and β process are observed in experiments above and below this temperature, respectively. Upon cooling through a dynamic crossover at ca. 175K, the dynamics of the liquid fraction becomes anisotropic and localized, implying solidification of the corresponding water network, most probably, during a confinement-affected glass transition.

[1] Mishima; *Nature*, Vol. 396, 329(1998)

CPP 13.2 Mon 15:15 ZEU 146

Understanding the nonlinear mobility of single driven parti-

cles in supercooled liquids — ●CARSTEN F. E. SCHROER^{1,2} and ANDREAS HEUER^{1,2} — ¹WWU Münster, Münster, Germany — ²Graduate School of Chemistry, Münster, Germany

We perform MD simulations of a binary Lennard-Jones mixture where a single particle is pulled by an external field through the liquid. Herein, we are specifically interested in the range of intermediate and strong forces when nonlinear effects occur in the single particle dynamics.

It is known from experimental and simulation studies, that the steady-state velocity \bar{v} follows in the limit of low forces a linear response relation $\bar{v} = \mu F$ where the force F is connected to the dynamical response via the constant mobility $\mu_0 = \frac{D_0}{k_B T}$. For large forces, however, one finds a dramatic increase of \bar{v} with increasing F , indicating a nonlinear force-dependence of the mobility, i.e. $\mu_0 \rightarrow \mu(F)$.

To gain a deeper understanding of this behavior, we studied the underlying potential energy landscape of the system by computing the minima the system has resided in during its time-evolution. This immediately allows us to discuss the nonlinear mobility in terms of thermodynamical (distribution of energies) and kinetic (escape rates out of single minima) quantities. Most interestingly it turns out, that both effects are of major importance for the nonlinearity of the system, so that there is no single nonlinear effect but an interplay of two independent which contributes to the dynamical responses of the driven particles.

CPP 13.3 Mon 15:30 ZEU 146

Simulation of Borate glasses — ●CHRISTOPH SCHERER^{1,2}, FRIEDERIKE SCHMID¹, MARTIN LETZ², and JÜRGEN HORBACH³ — ¹Johannes Gutenberg-Universität, Mainz — ²Schott AG, Mainz — ³Heinrich-Heine-Universität, Düsseldorf

The model glass former B₂O₃ is studied as an example for generating accurate glass structures on the computer. B₂O₃ is an important component for the simulation of oxide glasses since boron can form triangular planar structures, as well as tetrahedral nearest neighbor structures and also boroxol rings. In one approach, configurations of a few hundred atoms are equilibrated at high temperature, well above the glass transition temperature, with a classical molecular dynamics simulation (MD). After a quench down to 0K, they are structurally relaxed by means of an ab initio (DFT) calculation. The structural and vibrational properties are compared to the results of a full ab initio quench to 0K and to experimental results. The dependence of the glass structure and the liquid properties on the classical force field is examined. Therefore, a set of classical force fields is generated by means of a structural fitting procedure. The parameters are fitted in a way that the structure, namely the radial distribution functions and the angular distributions, of a classical MD run matches as closely as possible the structure of an ab initio (DFT) run at the same temperature. Parameter fits are carried out according to an ab initio trajectory at high temperature, where the system is in the liquid state. This sets the basis for the next steps: The development of a classical force field for sodium-borate glasses by the same methodology.

CPP 13.4 Mon 15:45 ZEU 146

Mixing random organization and jamming — ●MICHAEL SCHMIEDEBERG — Institut für Theoretische Physik 2: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40204 Düsseldorf, Germany

The random organization and the athermal jamming transition can both be studied in a unifying model system. We study the mixture of the protocols of the two transitions and argue that such a mixture can be interpreted as the glass transition at small but non-zero temperatures.

In our model system, first particles are randomly distributed and then in each step overlapping particles are displaced. In case of displacements in random directions the so-called random organization transition is observed. For purely deterministic displacements the jamming transition is realized. While the jamming protocol match with a quench of a soft sphere system from infinite to zero temperature without crossing energy barriers, the random displacements of the random organization protocol correspond to thermally activated rearrangements of particles. If in a mixed protocol the probability of random displacements is small but non-zero we find that the transition differs significantly from the purely deterministic jamming transition. We believe that our model system can help to understand why there is a difference between the glass transition at small but non-zero temperatures and the athermal jamming transition.

CPP 13.5 Mon 16:00 ZEU 146

Existence of glass-form factors — ●THOMAS FRANOSCH — Institut für Theoretische Physik, Leopold-Franzens-Universität Innsbruck, A-6020 Innsbruck, Austria

A hallmark of the glass transition is the slow structural relaxation of a quasi-arrested structure. As an idealization the dynamics is considered to become non-ergodic directly at the glass transition such that all auto-correlation function coupling to the structural relaxation exhibit finite non-trivial long-time limits often referred to as glass-form factors or nonergodicity parameters. Simultaneously, the theory of stochastic processes in the framework of probability theory imposes quite stringent conditions on the class of correlation functions. The existence of a finite limit at long times is then connected to the properties of the associated spectral measure, and in general correlation functions can either oscillate forever, display quasi-periodic behavior, or even intermittent behavior. While for purely relaxation dynamics, e.g. Brownian dynamics, the existence of a long-time limit is trivial, the situation for the case of Newtonian dynamics has been elusive so far.

In this talk I elaborate conditions covering a broad class of theoretical approaches that guarantee the existence of a long-time limit. As a special case I show that the mode-coupling theory of the glass transition belongs to that class. As an outlook I briefly discuss the case of multiple decay channels relevant for molecular or confined systems.

15 min break

CPP 13.6 Mon 16:30 ZEU 146

Spin freezing in geometrically frustrated magnets — JORGE REHN¹, ARNAB SEN^{1,2}, ●ALEXEI ANDREANOV¹, ANTONELLO SCARDICCHIO³, KEDAR DAMLE⁴, and RODERICK MOESSNER¹ — ¹Max-Planck Institut für Physik komplexer Systeme, Dresden, Germany — ²Indian Association for the Cultivation of Science, Kolkata, India — ³The Abdus Salam ICTP, Trieste, Italy — ⁴The Tata Institute, Mumbai, India

Materials which are believed to be faithfully represented by classical frustrated magnets with macroscopically degenerate groundstates, often exhibit spin-freezing. The latter is a transition to a spin-glass phase. Explaining the mechanism of such freezing is not always a simple task, since conventional ingredients, like randomness of the interactions, is not always present in the systems under study. We present a model, where dilution alone generates frustrating interaction between certain spins in the systems and leads to their freezing. The effective model deals with antiferromagnetically coupled Heisenberg spins in 2D. Both the long-range nature of the interaction and its dependence on the distance are crucial for the existence of the glass phase. We confirm our predictions by performing Monte-Carlo simulation of the effective model.

CPP 13.7 Mon 16:45 ZEU 146

Glasses of binary colloidal mixtures in the quiescent state and under shear — ●TATJANA SENTJABRSKAJA, MARCO LAURATI, and STEFAN EGELHAAF — Condensed Matter Physics Laboratory, Heinrich-Heine Universität Düsseldorf, D-40225 Düsseldorf, Germany

We investigate mixing effects on the glass state of binary colloidal hard sphere mixtures with large size asymmetry (size ratio 1:5). Increasing the amount of small spheres in a system of large ones, a glass-glass transition is observed, where the large particles, initially caged by the large spheres, become localised in a cage of small spheres [1]. During the transition, the dynamics accelerate and a strong reduction of the yield strain as a result of the shift of random close packing is observed [2].

The results of rheology are compared to measurements of the dynamics of particles under shear. The super-diffusion typically associated with stress overshoots [3] becomes more pronounced for mixtures in which the dynamics are increasingly arrested. Moreover, we observe different degrees of shear-induced constriction depending on mixing ratio, which closely follow changes in the magnitude of the stress overshoot.

- [1] T.Sentjabrskaja et al., AIP Conf.Proc., 1518, 206, 2013.
- [2] T.Sentjabrskaja et al., Soft Matter, 9(17), 4524- 4533, 2013.
- [3] M.Laurati et al., J. Phys.: Condens. Matter, 24, 464104, 2012.

CPP 13.8 Mon 17:00 ZEU 146

Microscopic theory for sheared colloidal glasses and gels — ●CHRISTIAN AMANN and MATTHIAS FUCHS — Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

We use mode coupling theory (MCT) to calculate in three dimensions (3D) transient density autocorrelators in start-up shear flow. It is thus possible to quantitatively predict flow curves and distorted structure of colloidal glasses and gels under shear flow. We investigate the transient, non-linear, non-monotonous stress response to strain and structure-factor distortion in 3D as well as steady-state flow curves (cf. [1] for 2D calculations). Density correlators, stress response, and structure-factor distortions are in good qualitative agreement with experiments [2], while the quantitative errors of the theory can be identified. A close connection between the time-evolution of symmetries of structure-factor distortions and non-monotonous stress response (i.e. stress overshoot) can be observed. We use as input a structure factor calculated with analytical Percus Yevick closure, which allows to approximate a hard sphere repulsion as well as augmenting a short range square-well attraction [3]. Hence, implications of a gel-glass to repulsive-glass transition on the transient rheology can be studied.

- [1] Amann, C.P. et al. *J. Rheol.* **57**, 149 (2013); Henrich O. et al. *Phil. Trans. R. Soc. A* **367**, 5033 (2009)
- [2] Denisov, D. et al. *Sci. Rep.* **3**, 1631 (2013)
- [3] Dawson K. et al. *PRE* **63**, 011401 (2000)

CPP 13.9 Mon 17:15 ZEU 146

An efficient Monte Carlo algorithm to study structural relaxation in network forming materials — ●RICHARD VINK — Institute of Theoretical Physics, Georg-August-Universität Göttingen, Germany

Network forming materials are ubiquitous in nature, common examples being semiconductors such as silicon and silica, as well as fluids that can form hydrogen bonds. What these materials have in common is that their topology on short length scales is governed by certain rules. For example, in amorphous silicon, most atoms are 4-fold coordinated, the preferred Si-Si bond length being ≈ 2.35 Å, and the preferred Si-Si-Si bond angle being the tetrahedral angle. This complicates molecular dynamics simulations of these materials, where the particles spend most of their time thermally fluctuating about their equilibrium positions, while large structural changes in the network topology are rare. To overcome this problem, Wooten, Winer, and

Weaire (WWW) introduced a special Monte Carlo move consisting of bond switching Monte Carlo moves which turned out to be very efficient at structurally relaxing networks of amorphous silicon and silica [Phys. Rev. Lett. **54** 1392 (1985)]. Unfortunately, the algorithm is only correct when used at zero temperature. In order to also address finite temperature, I propose a modification to the original WWW algorithm such that the Boltzmann distribution is faithfully sampled at any given temperature. The resulting algorithm is used to study the melting transition of a two-dimensional three-fold coordinated network.

CPP 14: Focused Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale II (original: O, joined by CPP)

Time: Monday 16:00–18:45

Location: TRE Ma

Topical Talk CPP 14.1 Mon 16:00 TRE Ma
Simulating heat transport: from large scale molecular dynamics to first-principles calculations — ●DAVIDE DONADIO — Max Planck Institute for Polymer Research, Mainz, Germany

The necessity to design materials and devices able to harness thermal energy, and possibly convert it into more amenable energy forms, has stimulated a major effort in the scientific community to understand heat transport at the mesoscale and the nanoscale. In this talk I will discuss different atomistic approaches to simulate nanoscale heat transport, ranging from large scale molecular dynamics simulations with classical empirical potentials at equilibrium and non-equilibrium conditions, to lattice dynamics calculations with force-constants computed by first principles. Applications will include silicon and carbon nanostructures, phase-change materials and molecular junctions.

CPP 14.2 Mon 16:30 TRE Ma
First principles study of thermal conductivity cross-over in nano-structured Zinc-Chalcogenides — ●ANKITA KATRE¹, ATSUSHI TOGO², RALF DRAUTZ¹, and GEORG K. H. MADSEN¹ — ¹ICAMS, Ruhr-Universität Bochum, 44801 Bochum, Germany — ²ESISM, Kyoto University, Sakyo, Kyoto 606-8501, Japan

Nano-structured Zinc-Chalcogenides are interesting for thermoelectric applications due to their low thermal conductivity.[1] A simple model study has reported how the thermal conductivity of ZnS, ZnSe and ZnTe can potentially show a cross-over as a function of the maximal mean free path of the phonons.[2] We have applied the Boltzmann transport equation in the relaxation time approximation to verify this. We find that thermal conductivity of ZnS crosses ZnSe and ZnTe and explain this in terms of the different contributions of phonon modes in these materials. Furthermore, the cross-over is found to be strongly influenced by isotope scattering. The calculated thermal conductivity is found to be strongly dependent on the volume and we explain the observed differences between LDA and GGA calculations. We compare further calculated thermal properties, such as the thermal expansion coefficient, to experiment to validate our approach.

[1] L.Zhen, S.Qiao, D.Y.Xiang, H.Z.Zhong, and Q.L.Gao, J. Mater. Chem. **22**, 22821 (2012). [2] N.Mingo and D.Broido, Phys. Rev. Lett. **93**, 246106 (2004).

CPP 14.3 Mon 16:45 TRE Ma
Density-functional perturbation theory for lattice dynamics with numeric atom-centered orbitals — ●HONGHUI SHANG, CHRISTIAN CARBOGNO, PATRICK RINKE, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der MPG, Berlin

The response of the electronic structure to atomic displacements gives rise to a variety of interesting physical phenomena, which can be probed by experimental techniques such as infrared or Raman spectroscopy or neutron diffraction. The response can be conveniently computed from first principles by means of density-functional perturbation theory (DFPT). Here we present our implementation in the all-electron atom-centered numeric orbital code FHI-aims [1]. Our approach combines the accuracy of an all-electron full-potential treatment with the computational efficiency of localised atom-centered basis sets that is necessary to study large and complex systems. We verified the accuracy of our DFPT implementation by comparing the vibrational frequencies to finite-difference reference calculations and literature values. Due to the atom-centered nature of the integration

grids in FHI-aims, the portion of the grid that belongs to a certain atom also moves when this atom is displaced. Here we demonstrate that, unlike for first derivatives (i.e. forces) [2], this moving-grid-effect plays an important role for second derivatives (i.e. vibrational frequencies). Further analysis reveals that predominantly diagonal force constant terms are affected, which can be bypassed efficiently by invoking translational symmetry.

- [1] V. Blum et al. Comp. Phys. Comm. **180**, 2175 (2009)
 [2] B. Delley, J. Chem. Phys. **94**, 7245 (1991).

CPP 14.4 Mon 17:00 TRE Ma
Breakdown of Fourier law in layered materials — ●ANDREA CEPELLOTTI¹, GIORGIA FUGALLO², FRANCESCO MAURI³, and NICOLA MARZARI¹ — ¹THEOS, École Polytechnique Fédérale, Lausanne — ²IMPMC, Université Pierre et Marie Curie, Paris — ³LSI, École Polytechnique, Paris

We compute the thermal conductivity in crystalline layered materials by solving the Boltzmann Transport Equation (BTE) for phonons [1], with the phonon-phonon collision rates obtained from density-functional perturbation theory. We find that in 2D materials, such as graphene and related compounds, and even in 3D layered materials, like bulk graphite, the single-mode relaxation time approximation (SMRTA) cannot describe heat transport correctly, underestimating by one order of magnitude or more thermal conductivities and phonons' mean free paths. Instead, we show that the exact self-consistent solution of the BTE provides results in excellent agreement with experimental measurements [2]. The shortcomings of the SMRTA lie in the assumption that heat flow is transferred only by individual phonon excitations, whereas in layered materials the transport can only be explained in terms of collective phonon excitations. The characteristic length of these collective excitations is often comparable with that of the experimental sample - as a result, Fourier's law become questionable, since its statistical nature makes it applicable only to systems larger than a few mean free paths.

- [1] G. Fugallo et al., Phys. Rev. B, **88**, 045430 (2013).
 [2] A. A. Balandin, Nat. Mater. **10**, 569 (2011).

CPP 14.5 Mon 17:15 TRE Ma
High Temperature Thermal Conductivity from First Principles — ●CHRISTIAN CARBOGNO¹, RAMPI RAMPRASAD², and MATTHIAS SCHEFFLER¹ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — ²Chemical, Materials & Biomolecular Engineering, University of Connecticut, Storrs, USA

In spite of significant research efforts, a first principles determination of the thermal conductivity at high temperatures has remained elusive. Under such conditions, Boltzmann transport techniques [1] that include anharmonic effects only perturbatively become inaccurate or even inapplicable. In this work, we overcome this limitation by performing first-principles Green-Kubo simulations [2], in which all orders of anharmonicity are incorporated by the means of *ab initio* molecular dynamics. The thermal conductivity is then assessed from the auto-correlation function of the heat flux in thermodynamic equilibrium. We discuss the details of our implementation and the definition of our heat flux that is based on the virial theorem. We validate our approach by presenting calculations for ZrO₂ that also showcase the importance of higher order anharmonic effects in materials with low thermal conductivities. Eventually, we discuss how our technique can

be coupled to multi-scale models to achieve a computationally efficient and accurate description of the thermal conductivity at the nanoscale.

[1] D. A. Broido *et al.*, *Appl. Phys. Lett.* **91**, 231922 (2007).

[2] R. Kubo, M. Yokota, S. Nakajima, *J. Phys. Soc. Jpn.* **12**, 1203 (1957).

CPP 14.6 Mon 17:30 TRE Ma

Accurate Modelling of the Polymorphism and Elastic Response of Molecular Materials from First Principles — ●ANTHONY REILLY and ALEXANDRE TKATCHENKO — Fritz-Haber-Institut der MPG, Berlin, Germany

Molecular materials are of great fundamental and applied importance in science and industry, with numerous applications in pharmaceuticals, electronics, sensing, and catalysis. A key challenge for theory has been the prediction of their stability, polymorphism and response to perturbations. While pairwise models of van der Waals (vdW) interactions have improved the ability of density functional theory (DFT) to model these systems, quantitative and even qualitative failures often remain. Here, we show how a many-body description of vdW interactions can dramatically improve the accuracy of DFT for molecular materials, yielding quantitative description of stabilities and polymorphism for these challenging systems. Moreover, the role of many-body vdW interactions goes beyond stabilities to response properties. In particular, we have studied the elastic properties of a series of molecular crystals, finding that many-body vdW interactions can account for up to 30% of the elastic response, leading to quantitative and qualitative changes in elastic behavior. We will illustrate these crucial effects with the challenging case of the polymorphs of aspirin, leading to a better understanding of the conflicting experimental and theoretical studies of this system.

CPP 14.7 Mon 17:45 TRE Ma

Surface chemistry on nanostructured oxides: do we have to go beyond hybrid DFT? — ●DANIEL BERGER, HARALD OBERHOFER, and KARSTEN REUTER — Technische Universität München, Germany

Nanostructured oxide surfaces are promising candidates for a wide range of energy and catalysis applications. For first-principles modeling of corresponding surface chemical reactions the current state-of-the-art is generally defined by hybrid-level density-functional theory (DFT). Systematic work assessing the achieved accuracy at this level is nevertheless scarce, also owing to the fact that higher-level reference methods are often not available for standard periodic boundary condition supercell calculations. To this end, we present a study benchmarking semi-local and hybrid DFT against (renormalized) second-order perturbation theory (MP2,rPT2) as recently implemented in the FHI-aims package [1]. We make the efficient usage of the latter theories for oxide surfaces possible through a solid-state embedding framework, in which a central cluster region is described quantum mechanically, the long-range electrostatic interactions in the oxide are accounted for through a polarizable monopole field, and a shell of norm-conserving pseudopotentials correctly connects the two regions. We illustrate the performance of the various levels of theories using the water-splitting reaction at ideal and defected TiO₂(110) surfaces as showcase. [1] X. Ren *et al.*, *Phys. Rev. B* **88**, 035120 (2013)

CPP 14.8 Mon 18:00 TRE Ma

Atoms-in-solids perspective on polarizabilities and van der Waals coefficients in semiconductors — ●GUO-XU ZHANG, ANTHONY M. REILLY, ALEXANDRE TKATCHENKO, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der MPG, Berlin, Germany

The calculation of response properties of solids including their polarizabilities and van der Waals (vdW) coefficients usually requires the knowledge of the full electronic bandstructure. For non-covalently bound solids, such as noble-gas and ionic crystals, atoms-in-solids model can be successfully utilized to define their polarizabilities. Here we critically assess the atoms-in-solids model for covalently-bound

solids, ranging from wide-gap (10 eV) to narrow-gap (below 1 eV) semiconductors. We model their response by assigning a single quantum harmonic oscillator to every atom, where the parameters of the oscillators are defined as functionals of the electron density, following the Tkatchenko-Scheffler method [1]. The response function is then calculated by solving self-consistent screening equations of classical electrodynamics, without any explicit information about the electronic bandstructure [2]. The calculated polarizabilities and vdW coefficients for 23 semiconductors are compared with TDDFT and experimental benchmark data, revealing an overall agreement within 10%. The efficiency of our method and the accuracy of the calculated vdW parameters allows us to demonstrate the crucial role of vdW interactions in the cohesive properties of the 23 semiconductors. [1] Tkatchenko and Scheffler, *PRL* (2009); [2] Tkatchenko, DiStasio, Car, Scheffler, *PRL* (2012).

CPP 14.9 Mon 18:15 TRE Ma

Adsorption at semiconductor surfaces - an energy analysis method — ●RALF TONNER and MARC RAUPACH — Fachbereich Chemie & Materials Sciences Centre, Philipps-Universität Marburg, Germany

The chemical bond is one of the most fundamental concepts in chemistry. Classifications such as covalent, ionic or metallic bonding are central in discussing trends in different compounds and predicting new reactivity. Several very helpful concepts and methods were developed to understand the chemical bond at surfaces.[1] The question about energetic contributions to surface chemical bonds on the other hand did not receive great attention although energy changes are the ultimate driving force in bond formation.

Starting from preliminary work by Philippsen and Baerends,[2] we implemented all terms of an Energy Decomposition Analysis (EDA) to obtain quantitative data about energetic contributions to chemical bonding in periodic systems. This periodic EDA method was applied to questions of chemisorption of organic molecules at semiconductor surfaces where it can shed light on the nature of the surface-adsorbate bonds.

[1] a) A. Nilsson, L. G. M. Pettersson, J. Nørskov, *Chemical Bonding at Surfaces and Interfaces*, Elsevier, Amsterdam, 2007; b) A. Groß, *Theoretical Surface Science*, Springer, Berlin, Heidelberg, 2009. [2] P. H. T. Philippsen, E. J. Baerends *J. Phys. Chem. B* 2006, 110, 12470.

CPP 14.10 Mon 18:30 TRE Ma

Non-local density functionals meet many-body dispersion: A hybrid approach for van der Waals interactions — ●JAN HERMANN, MATTHIAS SCHEFFLER, and ALEXANDRE TKATCHENKO — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Different approaches to treating van der Waals (vdW) interactions in density-functional theory can be loosely divided into the atom-based and the ones based on non-local functionals. The first type comprises a range of methods from atom-pairwise additive schemes by Grimme to many-body dispersion (MBD) approach of Tkatchenko et al. Usually, these methods require precalculated atomic parameters and thus rely on information not explicitly contained in the electron density. The other category consists of nonlocal functionals either of the Langreth and Lundquist or the Vydrov and van Voorhis (VV) type. In these approaches, the vdW interaction is obtained as a functional of the electron density and at most a few tuning parameters are needed.

Here, we show that these two contrasting approaches can be synergistically combined. We use the polarizability from the nonlocal functional of VV within the MBD method of Tkatchenko et al. Such a combination is worthy for several reasons. First, it is an atom-centered approach with no atomic parameters. Second, it puts aside the problem of partitioning electron density between atoms, which can be problematic in some cases. Third, it enables more direct comparison of so far unrelated methods. Fourth, it highlights the idea of combining working elements from different approaches.

CPP 15: Organic Electronics and Photovoltaics A (original: DS, joined by CPP, HL, O)

Time: Monday 18:00–19:45

Location: CHE 91

CPP 15.1 Mon 18:00 CHE 91

Studying the electric potential of organic solar cells — ●MICHAEL SCHERER^{1,2,3}, TOBIAS JENNE^{1,2,3}, REBECCA SAIVE^{1,2,3}, FELIX SCHELL^{1,2,3}, ROBERT LOVRINCIC^{1,2,3}, and WOLFGANG KOWALSKY^{1,2,3} — ¹InnovationLab GmbH, Heidelberg — ²TU Braunschweig — ³Universität Heidelberg

Despite steadily increasing efforts in the research on organic semiconductors, many of the models applied in the field are restricted to small clusters of molecules or model systems only, thus lacking prediction when it comes to full devices. With scanning Kelvin probe microscopy (SKPM) accompanied by device simulations we try to access the physics of entire OSC devices and bridge the gap between the molecular and the macroscopic understanding.

Our scanning probe station is placed within the vacuum of a scanning electron microscopy (SEM)/focused ion beam (FIB) cross beam system. We prepare OSC cross sections with the FIB and place the cantilever under SEM observation right at the cross section. Thus we are able to investigate the potential distribution of OSCs in situ with SKPM.

The SKPM measurements are backed by IV characterization and device simulations. Varying the parameter of the active layer/contact interface, we investigate their impact on the potential distribution and the device characteristics of the OSC. In IV measurements and cross sectional SKPM measurements we check the validity of the applied models and identify loss mechanisms and their localization in the solar cell device.

CPP 15.2 Mon 18:15 CHE 91

Correlation of electric properties and interface band alignment in organic light-emitting diodes — ●MAYBRITT KÜHN^{1,2}, ERIC MANKEL^{1,2}, CHRISTOF PFLUMM³, THOMAS MAYER^{1,2}, and WOLFRAM JAEGERMANN^{1,2} — ¹Technische Universität Darmstadt, Institute of Materials Science, Surface Science Division — ²InnovationLab GmbH, Heidelberg — ³Merck KGaA, Darmstadt

Organic light-emitting diodes consist of several functional organic layers sandwiched between two electrodes with different work functions. At the current onset voltage the applied electric field is high enough that charge carrier injection and transport begins. In some device structures the onset voltage increases with increasing thickness of the emission layer. We present a detailed study on this up to now unpredictable phenomenon by combining IV-measurements and interface investigations using photoelectron spectroscopy (XPS/UPS). We focus on two isomers synthesized by Merck that serve as matrix material in the emission layer—one showing the changes in onset voltage the other not. The complex device architecture was reduced to a model device system using NPB as hole-transport layer and the undoped isomers as emission layer. The shift in onset voltage can still be observed in the model devices as well in hole-only devices derived from the model system. By stepwise evaporation of the respective isomer onto NPB we performed PES-interface experiments and analyzed the band alignment between NPB and the isomers in an integrated UHV system. It was found that the hole injection barrier is larger by about 200 meV in case of the isomer showing the observed shift in onset voltage.

CPP 15.3 Mon 18:30 CHE 91

Temperature dependent exciton diffusion length in ZnPc — ●BERNHARD SIEGMUND¹, JOHANNES WIDMER¹, SIMONE HOFMANN¹, MORITZ RIEDE², and KARL LEO¹ — ¹Institut für Angewandte Photophysik, Dresden, Germany — ²Current address: Clarendon Laboratory, Oxford, England

The photo-current of organic solar cells is the result of a multi-step process. It includes the generation and diffusion of excitons as well as their separation into free charge carriers, the transport to the electrodes, and their final extraction. One bottleneck for highly efficient devices is the short exciton diffusion length in organic materials.

In this work, the singlet exciton diffusion length ℓ_{diff} in the absorber material ZnPc is studied. For this purpose, the photo-current of organic solar cells, incorporating ZnPc and C₆₀ in a flat heterojunction architecture, is measured and modelled as a multi-step process. ℓ_{diff} is extracted from a thickness variation of the absorber layer, as not yet encountered in the context of modelling the photo-current to determine ℓ_{diff} before. Measurements at varying temperature between 200 K and

370 K reveal a thermal activation of the diffusion length above 310 K. This is interpreted as promotion of the excitons to higher energies with a density of states allowing for enhanced hopping transport. The activation energy is considered as a measure for the energetic disorder of the excitonic states. These investigations aim for a better understanding of exciton migration in order to design materials with longer exciton diffusion lengths for highly efficient organic solar cells.

CPP 15.4 Mon 18:45 CHE 91

The effect of gradual fluorination on the opto-electronic properties of F_nZnPc/C₆₀ bilayer cells — ●M. BRENDEL¹, A. STEINDAMM¹, A. TOPCZAK¹, and J. PFLAUM^{1,2} — ¹Exp. Phys. VI, JMU Würzburg, 97074 Würzburg — ²ZAE Bayern, 97074 Würzburg

The respective position of energy levels at the donor/acceptor heterojunction is crucial for the resulting parameters of an organic solar cell. For instance the open circuit voltage (V_{oc}) is correlated to the energy difference between the highest occupied molecular orbital (HOMO) of the donor and the lowest unoccupied molecular orbital (LUMO) of the acceptor, the so-called effective band gap ($E_{g,eff}$). To gain insights into this correlation, tailoring of energy levels by chemical modification is a powerful approach. In this contribution, we investigate the impact of gradual fluorination of zinc phthalocyanine on the opto-electronic properties of F_nZnPc/C₆₀ (n=0,4,8,16) bilayer cells. Upon fluorination, HOMO and LUMO levels are shifted towards lower energies. The gain in V_{oc} for F₄ZnPc/C₆₀ and F₈ZnPc/C₆₀ by 11% and 23% respectively, compared to ZnPc/C₆₀, confirms qualitatively the expected energy level scheme. Besides, the differences between $e \cdot \Delta V_{oc}$ and $\Delta E_{g,eff}$ hint at the occurrence of dipoles and their gain in strength with increasing degree of fluorination. As will be shown, this dipol can be correctly accounted for in a plate capacitor geometry, considering image charges at the interface induced by electronegative fluorine in the immediate vicinity of C₆₀ molecules. We thank S. Sundarray and P. Erk from BASF for providing F₄ZnPc. Financial support by the DFG (program SPP1355) and the BMBF (GREKOS program).

CPP 15.5 Mon 19:00 CHE 91

Effect of Counter-Anions During Electrodeposition on the Charge Transport Dynamics in Sensitized ZnO Solar Cells — ●CHRISTOPH RICHTER, MAX BEU, and DERCK SCHLETTWEIN — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany

Thin porous ZnO/EosinY films have been electrochemically deposited from oxygen-saturated aqueous solution. During the electrochemical deposition chloride or perchlorate as different counter-anions have been used. After the removal of EosinY with KOH the films have been sensitized with the indoline dye D149. These electrodes were used in dye-sensitized solar cells (DSCs) and the charge transport dynamics were studied with electrochemical impedance spectroscopy (EIS), intensity modulated current/voltage spectroscopy (IMPS/IMVS) and IV-curves. Doping of the ZnO films by Cl alters the charge transfer dynamics by filling of otherwise unoccupied states in ZnO and changing the concentration of available trap states. By changing the counter-anion to perchlorate well-reproducible results could be obtained which open the way to further improvements in DSCs.

CPP 15.6 Mon 19:15 CHE 91

Efficiency roll-off in organic light-emitting diodes: influence of emitter position and orientation — ●CAROLINE MURAWSKI¹, PHILIPP LIEHM^{1,2}, SIMONE HOFMANN¹, KARL LEO¹, and MALTE C. GATHER^{1,2} — ¹Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — ²present address: SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews KY16 9SS (UK)

In this contribution, we study the efficiency decrease of organic light-emitting diodes (OLEDs) at high brightness (so-called roll-off).[1] We find a strong influence of the emitter-cathode distance and the transition dipole orientation of the emitter molecules on the roll-off by comparing two phosphorescent emitters (Ir(MDQ)2(acac) and Ir(ppy)3).[2] The measurements are modeled using triplet-triplet-annihilation (TTA) theory. A comparison of experiment and theory reveals the critical current density and the TTA rate constant and shows that the differences in roll-off behavior are predominantly caused by a change of the decay rates inside the OLED cavity. In order to

provide guidelines for designing OLEDs with optimal high-brightness efficiency, we model the roll-off as a function of the emitter-cathode distance, emitter dipole orientation, and radiative efficiency.

[1] C. Murawski, K. Leo, and M.C. Gather, *Adv. Mater.* 10.1002/adma.201301603 (2013).

[2] C. Murawski, P. Liehm, K. Leo, and M.C. Gather, *Adv. Funct. Mater.* 10.1002/adfm.201302173 (2013).

CPP 15.7 Mon 19:30 CHE 91

Solution-based planarization layers for organic solar cells on flexible silver nanowire transparent electrodes — ●JAN LUDWIG BORMANN¹, FRANZ SELZER¹, NELLI WEISS², LARS MÜLLER-MESKAMP¹, and KARL LEO¹ — ¹Institut für Angewandte Photophysik, TU Dresden — ²Physikalische Chemie, TU Dresden

Flexible transparent electrodes made of silver nanowires (AgNWs) are

an emerging research field for different optoelectronic devices such as organic transistors, organic light emitting diodes (OLED) and organic photovoltaics (OPV). They exhibit excellent electrical and optical properties (sheet resistance of 11 Ohm/sq at 85% transmittance) and are suitable for the application on flexible substrates. These transparent electrodes show high roughness and therefore require a planarization layer for fabricating efficient small molecule devices.

In this work, solution-based organic materials are processed with spin coating to planarize the AgNW electrode. A solution processed small molecule layer acts as planarizing layer and as hole transport layer in organic solar cells with a bulkheterojunction comprising the fullerene C60 as acceptor and different small molecule donor layers (oligothiophenes and phthalocyanines). The efficiency of these devices is comparable or even better to reference devices with indium tin oxide (ITO) as transparent electrode.

CPP 16: Interfaces and Thin Films II

Time: Tuesday 9:30–13:00

Location: ZEU 114

CPP 16.1 Tue 9:30 ZEU 114

Lipid Monolayers and Adsorbed PSS with Different Degrees of Polymerization: Evidence of Lipid/PSS Complexes — ●THOMAS ORTMANN, HEIKO AHRENS, ANDREAS GRÖNING, FRANK LAWRENZ, and CHRISTIANE A. HELM — Inst. f. Physik, Uni Greifswald, 17487 Greifswald, Germany

To gain insight into the equilibrium conformation of adsorbed polyelectrolytes and into their interactions with the supporting surface, lipid monolayers at the air/water interface serve as model substrate with adjustable surface charge.

Monolayers of cationic lipid DODA with adsorbed anionic Polystyrene sulfonate (PSS) are studied by isotherms and X-ray techniques. From salt-free solutions, PSS adsorbs flatly. The lipid monolayer shows a fluid/ordered phase transition. For polymer lengths exceeding 8 nm, PSS adsorbs in a lamellar manner to the lipid monolayer, for both lipid phases. On monolayer compression, the area per lipid molecule and the intermolecular separation of the PSS chains are reduced by a factor of two. On increase of PSS molecular weight, the phase transition pressure of the lipids decreases until the polymer length exceeds the persistence length (27 nm), then it levels off. However, the phase transition enthalpy of the lipids is almost independent of PSS molecular weight. These observations suggest complexes consisting of stiff PSS chains and lipids. If the PSS chains are shorter than 8 nm, the lamellar arranged PSS chains are only found when the lipids are in the ordered phase.

CPP 16.2 Tue 9:45 ZEU 114

Electrostatic nanotemplates: A universal platform for controlled hierarchical particle-deposition. — ●TOM WAGNER, LARISSA TSARKOVA, and ALEXANDER BÖKER — Chair of Macromolecular Materials and Surfaces / Interactive Materials Research DWI an der RWTH Aachen e.V.

We target nanoscopically functionalized surfaces with potential applications in catalysis, circuitry, molecule-recognition and optoelectronics. Nanocomposite templates with topographically and chemically structured patterns have been prepared using a physicochemical bottom-up technique. As a basic nanopattern we use thin films of microphase separated diblock copolymers, aligned by the application of an electric field. The introduction of positive charges exclusively into one particular block is achieved via inter/intra molecular crosslinking, providing a manifold usable electrostatic nanotemplate. Further, microcontact printing and dipcoating processes allow the selective adsorption of negatively charged nanoparticles, proteins and polyelectrolytes, in order to obtain periodic superstructures. In the course of structuring, the degree of crosslinking (charge-density) as well as the elemental composition of precursors and of the final composites has been monitored by attenuated total reflection infrared spectroscopy (ATR-IR) and by x-ray photoelectron spectroscopy (XPS). AFM- and FESEM-measurements have been used to characterize the topography and particle-arrangement at the composite surface. X-ray reflectivity (XRR) measurements provided information on the inner structure of the film.

CPP 16.3 Tue 10:00 ZEU 114

Scaling theory for compressed polymer-brush bilayers — ●TORSTEN KREER — Leibniz Institut für Polymerforschung Dresden, 01069 Dresden, Germany

When linear macromolecules are grafted densely onto a surface, the individual chains are forced to stretch away from the surface plane forming a polymer brush. Polymer brushes allow one to tune surface properties by modification of the functionality or the molecular parameters, i.e., chain length and density of the grafted chains. Thus, they are important in many respects, e.g. for the stabilization of colloidal dispersions, flocculation, wetting phenomena, and (bio-)lubrication. Of particular interest are two polymer brushes compressed against each other (so-called "polymer-brush bilayers"), which play an important role as model systems, e.g. to study biolubrication. Starting from the classical concepts to calculate the interaction free energy of such bilayers, known as the famous theory of Milner, Witten, and Cates and the scaling approach of Alexander and de Gennes, an alternative picture is developed that describes both numerical and experimental data significantly better. To this extent, basic scaling theory and the strong-stretching limit of the self-consistent mean-field theory will be discussed.

CPP 16.4 Tue 10:15 ZEU 114

Investigation of stretching and force-induced desorption of polymer chain anchored to repulsive and inert surfaces — ●ZORYANA USATENKO — Cracow University of Technology, 30-084 Cracow, Poland

The investigation of stretching and force-induced desorption of ideal and real polymer chain with excluded volume interactions in a good solvent anchored to repulsive and inert surface are performed. The calculations of the stretching and desorption force applied to free end of real polymer chain anchored by other end to repulsive and inert surface are performed up to one-loop order of the massive field theory approach in fixed space dimensions $d=3$. The obtained results are in good agreement with previous theoretical results obtained for the stretching force in "Z" ensemble calculated for the case of ideal chain anchored to the surface and have important practical applications for understanding of the elastic properties of the individual macromolecules, networks, gels and brush layers. Besides, the obtained in the framework of the massive field theory approach results are in good agreement with results of density functional theory approach for the region of small applied forces.

CPP 16.5 Tue 10:30 ZEU 114

POLARIZED μ -RAMAN IMAGING SPECTROSCOPY: CRYSTALLINITY AND ORIENTATION OF SHEARED PP FILMS — ●KRISZTINA VINCZE-MINYA¹, SABINE HILD¹, SIBYLLE JILG², and REINHARD FORSTNER² — ¹Institut für Polymerwissenschaften, Johannes Kepler Universität Linz, Österreich — ²TCKT Wels, Österreich

Isotactic PP ring-samples where prepared by Pirouette-dilatometer under different pressures and sheared at different temperatures and shear rates. The variations in crystallinity and orientation can be characterized on the microscale using polarized confocal Raman microscopy. For these investigations a method was developed previously by measuring

materials with known orientation (iPP thin films), whereby the results were correlated with WAXS. The good agreement of the Raman results with the WAXS-data was already reported in case of the defined samples. By the means of these findings the investigation method can be applied for the characterization of the samples with undefined orientation prepared with the Pirouette dilatometer.

CPP 16.6 Tue 10:45 ZEU 114

Studying polymer thin films with GISAXS contrast matching at the silicon K-edge — ●JAN WERNECKE¹, HIROSHI OKUDA², and MICHAEL KRUMREY¹ — ¹Physikalisch-Technische Bundesanstalt, Berlin, Germany — ²Kyoto University, Kyoto, Japan

Grazing-incidence small-angle X-ray scattering (GISAXS) is an ideal tool to study self-organized nanostructures in block-copolymer thin films as it allows for non-destructive, depth-resolved measurements. However, the strong scattering contribution of the film-substrate interface often makes the evaluation of weak scattering features of nanostructures within the film challenging. The reflection can be minimized by matching the scattering contrast of film and substrate to make the interface virtually 'invisible' for the X-ray beam. The most widely used substrate material is silicon. This requires to record scattering images in vacuum at around 1.8 keV, which is inaccessible for most digital large-area X-ray detectors. The performance of a newly developed in-vacuum PILATUS 1M detector¹ that can be operated down to 1.75 keV is shown in this presentation. The device is used to study structural changes in self-organized PS-b-P2VP thin films under the contrast matching condition at 1827 eV. Depth-resolved GISAXS measurements of the unperturbed scattering features of as-prepared and annealed films are presented and may offer further insights into thermally induced structural modifications along the PS-b-P2VP film thickness.

¹J Wernecke, C Gollwitzer, P Müller & M Krumrey: *Characterization of an in-vacuum PILATUS 1M detector*, submitted to *J. Synchrotron Rad.* (2013) arXiv:1311.5082.

15 min. break

CPP 16.7 Tue 11:15 ZEU 114

An X-ray reflectivity set-up for the study of solid/liquid interfaces under high hydrostatic pressure — FLORIAN J. WIRKERT, ●JULIA NASE, BENEDIKT NOWAK, IRENA KIESEL, SIMON KUJAWSKI, JOHANNES MÖLLER, PAUL SALMEN, MICHAEL PAULUS, CHRISTIAN STERNEMANN, and METIN TOLAN — Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund Germany.

Studying the response of matter to high hydrostatic pressure (HHP) has a long tradition. The knowledge on life at extreme conditions can be broadened if biological systems are investigated under HHP. The importance for studying biological systems at conditions up to 5 kbar lies also in the fact that biologically relevant proteins denature in this pressure regime.

We present the first set-up for in situ X-ray reflectivity studies (XRR) of solid/liquid interfaces at HHP up to 5 kbar [1]. With this new set-up, it is now possible to examine a number of different solid/liquid interfaces under HHP with Angström-resolution. In addition, the influence of a modified water structure (under HHP) on interfaces can be explored.

We present results concerning the structure of hydrophobic interface between OTS and water and discuss first XRR measurements of pressure-induced lysozyme adsorption on hydrophobic silicon wafers. The results demonstrate the enormous potential of the set-up, particularly for the study of biological systems.

[1] F. Wirkert et al, XRR measurements of liquid/solid interfaces at HHP conditions, *J. Synchr. Rad.* 21 (2014)

CPP 16.8 Tue 11:30 ZEU 114

Decontamination of lipophilic hazardous materials on sorptive solid surfaces — SALOMÉ VARGAS RUIZ¹, CHRISTOPH SCHULREICH², REGINE VON KLITZING¹, MARTIN JUNG³, THOMAS HELLMWEG², and ●STEFAN WELLERT¹ — ¹Stranski Laboratory, Technical University Berlin, 10623 Berlin, Germany — ²Physical Chemistry III, University Bielefeld, 33615 Bielefeld, Germany — ³Armed Forces Scientific Inst. f. NBC Protection, 29633 Munster, Germany

Modern decontamination media are desired to reconstitute personnel and equipment rapidly. The ability to extract penetrating hydrophobic surface hazards (e.g. pesticides, chemical warfare agents) out of sorptive surfaces and to instantaneously decompose the solubilized com-

pounds is essential. Microemulsions based on natural surfactants and plant and food grade oils possess a soft and "green" performance in a wide temperature range. Additionally, enzymatic degradation of highly toxic organophosphorus compounds inside microemulsions by the enzyme Diisopropyl fluorophosphatase (DFPase) was monitored. The microemulsion structure in the vicinity of model surfaces was investigated by neutron reflectometry. With respect to the desired functionalities, we discuss extraction properties and wetting behaviour of different microemulsions on model and realistic surfaces. Hence, the investigated systems are promising novel environmentally friendly extraction and reaction media providing interesting properties e.g. for biotechnological applications.

CPP 16.9 Tue 11:45 ZEU 114

Tuning the mechanical properties of ultrathin carbon nanomembranes via molecular design — ●XIANGHUI ZHANG¹, POLINA ANGELOVA¹, CHRISTOF NEUMANN¹, ANDRÉ BEYER¹, JÜRGEN SCHNACK², and ARMIN GÖLZHÄUSER¹ — ¹Physics of Supramolecular Systems and Surfaces, University of Bielefeld, Universitätstr. 25, 33615 Bielefeld — ²Condensed Matter Theory Group, University of Bielefeld, Universitätstr. 25, 33615 Bielefeld

Self-assembled monolayers (SAMs) of polyaromatic molecules can be cross-linked via low energy electron irradiation and form carbon nanomembranes (CNMs) with a thickness ranging from 0.5 to 3 nm. Freestanding CNMs were fabricated by transferring them onto a Si substrate with an array of orifices and an in-situ bulge test in an atomic force microscope (AFM) was used to characterize mechanical properties of CNMs. A differential pressure was applied to a freestanding CNM and the deflection at the centre of the membrane was recorded by AFM. We observe that the structure of precursor molecules has some effect on the mechanical stiffness of CNMs: CNMs from more rigid condensed polyaromatic precursors like naphthalene and pyrene thiols exhibit higher Young's moduli of 16-18 GPa; CNMs from non-fused oligophenyl molecules like biphenyl and terphenyl thiols possess lower Young's moduli of 8-10 GPa; CNMs from non-condensed hexaphenylbenzene and hexabenzocoronene thiols possess Young's moduli of 13-15 GPa. Finite element method (FEM) was also used to examine the deformation profiles and simulate the pressure-deflection relationship.

CPP 16.10 Tue 12:00 ZEU 114

Unexpected swelling characteristics of thermoresponsive polymer brush systems based on Poly(2-oxazoline)s — ●STEFAN ADAM^{1,2}, KLAUS-JOCHEN EICHHORN¹, JUAN CARLOS RUEDA³, MANFRED STAMM^{1,2}, MATHIAS SCHUBERT⁴, and PETRA UHLMANN¹ — ¹Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany — ²Technische Universität Dresden, 01062 Dresden, Germany — ³Pontificia Universidad Católica del Perú, Lima, Peru — ⁴University of Nebraska-Lincoln, Lincoln, NE 68588, USA

Responsive polymer coatings or hydrogels are capable to change their structural and physical properties due to changes in the environmental condition (e.g. temperature). Poly(2-oxazoline)s (POX), being structural isomers to polyacrylamides (e.g. poly(N-isopropylacrylamide), PNIPAAm) can exhibit a lower critical solution temperature (LCST) in aqueous solution. Adjusting the molar mass or copolymerization with more hydrophilic/hydrophobic comonomers enables tuning the LCST towards higher/lower temperatures. A combinatorial Quartz Crystal Microbalance with Dissipation and Spectroscopic Ellipsometry setup was used to study quantitatively the swelling characteristics of POX brushes prepared by the "grafting to" method using pre-synthesized polymers with functionalized end groups. The swelling behavior of POX brushes was compared to the phase transition of a corresponding aqueous polymer solution, determined by turbidity measurements. While all POX solutions show sharp transition curves in aqueous solution, an unexpected continuous reversible swelling of grafted POX could be observed over a wide temperature range.

CPP 16.11 Tue 12:15 ZEU 114

Hierarchical multiscale modelling of polystyrene-gold interfaces — ●KAREN JOHNSTON¹, VAGELIS HARMANDARIS², and KURT KREMER³ — ¹Department of Chemical and Process Engineering, University of Strathclyde, Glasgow, United Kingdom — ²Department of Applied Mathematics, University of Crete, Heraklion, Greece — ³Max Planck Institute for Polymer Research, Mainz, Germany

Polystyrene films between two parallel gold surfaces were studied using hierarchical multiscale modelling. Classical all-atom (AA) polymer-surface interface potentials were developed based on density functional theory calculations that account for van der Waals forces [1]. AA

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 (CG) model was used [3] and the CG surface potentials were developed based on all-atom potential of mean force calculations. The structural properties of the CG and AA simulations were compared for a 5 nm film of 10mer polystyrene and the results were in good agreement. The CG model was used to simulate 10 and 20 nm films for chain lengths of up to 200mer and the dependence of the structure and interphase width on chain length were investigated [4]. The effect of the CG interface potentials on the polymer dynamics near the surface will be discussed.

[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) [4] Johnston and Harmandaris, *Macromolecules*, 46, 5741 (2013)

CPP 16.12 Tue 12:30 ZEU 114

Monte Carlo study of polymer adsorption on nanocylinders — JONATHAN GROSS¹ and MICHAEL BACHMANN² — ¹Universität Leipzig, Leipzig, Germany — ²The University of Georgia, Athens, GA, USA

The thermodynamic behavior of a coarse-grained flexible polymer model in the vicinity of an attractive nanocylinder is subject of this investigation. We are interested in the structural phases of the polymer and how they change with the surface attraction strength of the nanocylinder. The effective monomer-surface attraction strength is associated with the cylinder radius and its material. Previous studies of polymer adsorption on planar surfaces already provide insight in the structures formed by adsorbed polymer chains. Recently also the ad-

sorption on curved surfaces was investigated. We try to connect the results of the adsorption on curved and planar surfaces, since in the limit of an infinite radius of the cylinder, the surface has the same characteristics as a plane. We construct complete pseudo-phase diagrams of a 30-mer interacting with nanocylinders of five different materials as a function of temperature and radius of the cylinders.

CPP 16.13 Tue 12:45 ZEU 114

Morphology, Mechanical Stability and Protective Properties of Ultrathin Gallium Oxide Coatings — FRANK LAWRENZ¹, PHILIPP LANGE², NIKOLAI SEVERIN², JÜRGEN P. RABE², CHRISTIANE A. HELM¹, and STEPHAN BLOCK³ — ¹Inst. f. Physik, Uni Greifswald, 17487 Greifswald, Germany — ²Dept. of Physics, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — ³Chalmers University of Technology, Gothenburg, Sweden

Scanning Force Microscopy (SFM) imaging of surfaces treated with liquid gallium shows extended, ultrathin layers, which are attributed to gallium oxide (GaOx) films. These 3 nm thick GaOx layers exhibit high mechanical stability as can be concluded from large forces required to rupture them with the SFM tip. We investigate the permeability of the films to oxygen and water. For this we cover fluorescent thin films made of conjugated polymers with the GaOx layers and investigate the degradation of fluorescence under ambient conditions. We estimated the upper limit of oxygen and water permeation rate of 0.06 molecules/day, this complies with the industrial requirements onto permeation barriers. Similar to other highly functional materials like graphene ultrathin GaOx layers could also be used for prospective transparent barrier applications.

CPP 17: Transport and Confinement I

Time: Tuesday 9:30–12:45

Location: ZEU 260

Invited Talk CPP 17.1 Tue 9:30 ZEU 260
Glassy dynamics of polymers in geometrical confinement: From nanometric layers to condensed isolated chains — FRIEDRICH KREMER — Institute of Experimental Physics I, University of Leipzig

The question on what length-scale molecular and especially glassy dynamics of polymers takes place is of fundamental importance and has multifold practical implications as well. Recent results based on Broadband Dielectric Spectroscopy for nanometric thin (>5 nm) layers of poly(styrene), poly(methylmethacrylate) and poly(cis-1,4-isoprene) will be presented, delivering the concurring result that deviations from glassy dynamics of the bulk never exceed margins of +/-3 K independent of the layer thickness, the molecular weight of the polymer under study and the underlying substrate. A further exciting perspective is the measurement of the dynamics of condensed isolated polymer chains. - The experiments lead to the conclusions that glassy dynamics takes place on the length-scale a few polymer segments (<0.5 nm) while the conformation of the chain as a whole is strongly modified due to geometrical confinement.

References: Tress, M. et al., *Science* 341, (6152) 1371-1374 (2013); Mapesa, E.U. et al., *Soft Matter* 9 (44), 10592-10598 (2013); Kremer, F., E.U. Mapesa, M. Tress, M. Reiche, "Molecular Dynamics of Polymers at Nanometric Length Scales: From Thin Layers to Isolated Coils" in: "Recent Advances in Broadband Dielectric Spectroscopy", Y. P. Kalmykov (Eds.), NATO Science for Peace and Security Series B: Physics and Biophysics, Chapter 12, Springer (2012)

CPP 17.2 Tue 10:00 ZEU 260

Direct measurement of thermophoretic forces — LAURENT HELDEN¹ und CLEMENS BECHINGER^{1,2} — ¹2. Physikalisches Institut, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — ²Max Planck Institut für Intelligent Systems, Heisenbergstr. 3, 70569 Stuttgart, Germany.

Thermophoretic motion of colloidal particles is ubiquitous in nature where ever temperature gradients occur. In spite of this the exact mechanism of thermophoretic motion is not yet fully understood and even preminent features like the size dependence of Soret coefficient are still under debate.

In this context we present a new strategy to directly measure thermophoretic forces. Using total internal reflection microscopy (TIRM)

we observe the motion of a single polystyrene particle in a narrow slit subjected to temperature gradients. With increasing gradient a preference of the cold side is observed. Implications for the theoretical description of thermophoresis are discussed.

CPP 17.3 Tue 10:15 ZEU 260

Anomalous Diffusion of Proteins in a Membrane due to Crowding and Trapping — MISLAV CVITKOVIĆ¹, TIMO BIHR^{1,2}, and ANA-SUNČANA SMITH¹ — ¹Institute for Theoretical Physics I and Cluster of Excellence: Engineering of Advanced Materials, Friedrich-Alexander-University Erlangen-Nürnberg (FAU), Germany — ²II Institute for Theoretical Physics, University of Stuttgart, Germany

The transport of lipids and proteins in biological membranes is one of the most fundamental processes in living cells. Despite a wealth of experiments on related biological processes, the general biophysical principles underlying the complex diffusion in a membrane are still not well understood. Here we model anomalous diffusion in the crowded and multicomponent membrane environment where proteins acting as tracers bind and unbind from immobilized counter-partners (traps), the latter representing a functionalized scaffold. Using a self-developed Monte-Carlo simulation scheme that accounts for length scales from 1 nm to 1 μm in the time domain from 1 μs to 10 s, we explore the full parameter space spanned by the densities of the diffusing molecules and the traps, as well as the binding and unbinding rates. We find several regimes of diffusion and types of anomalous transport. We determine the effective diffusion constant within an analytical model based on scaling arguments that account for trapping, self-avoidance and cooperative effects in the long-time limits of all regimes. We find that this approach reproduces well the results of analogous single-particle-tracking experiments in supported scaffolding membranes.

CPP 17.4 Tue 10:30 ZEU 260

Confinement of DGEBA: molecular dynamics & macroscopic flow — ANNA DJEMOUR, JOERG BALLER, CARLO DIGIAMBATTISTA, and ROLAND SANCTUARY — Laboratory for the Physics of Advanced Materials, University of Luxembourg, 162A, Avenue de la Faiencerie, L-1511 Luxembourg

Glass formers in confinement have been extensively studied with differing results: shifting of T_g towards smaller/higher temperatures, no shift, broadening of the glass transition, even several T_g s. This strongly depends on the type of confinement, the materials involved

and the confining surfaces and their treatment. These shifts can be used to determine the size of the cooperative rearranging regions aiding in the research into the nature of the glass transition. Additionally, there has been some work done on the influence of the confined matter on confining systems such as porous glasses (Ref. 1).

Both aspects were investigated for the low molecular weight epoxy resin DGEBA confined by a 3D porous network i.e. controlled pore glass with randomly oriented pores (native and silanized pores of pore sizes ranging from 4nm to 110nm). For native pores a large shift to higher temperatures was observed for the glass transition in small pores ($d \leq 20$ nm). Contributions from a layer adhered to the pore walls could be distinguished from a faster core layer of the glass former. We also observe a hitherto unreported hysteresis in heating and cooling measurements which we assume to be an effect of the macroscopic flow/transport of the glass former through the glass channels.

1. J. Koppensteiner et al, Phys. Rev. B 81 (2010) 024202.

CPP 17.5 Tue 10:45 ZEU 260

Hydrodynamic interactions induce anomalous diffusion under partial confinement — ●JOHANNES BLEIBEL^{1,2}, ALVARO DOMINGUEZ³, and MARTIN OETTEL¹ — ¹Institut für angewandte Physik, Universität Tübingen, Tübingen, Germany — ²Max-Planck-Institut für intelligente Systeme, Stuttgart, Germany — ³Física Teórica, Universidad de Sevilla, Sevilla, Spain

We consider a system of colloidal particles which are restricted to a plane, but surrounded by an unbound fluid. Examples for such a setup are colloids trapped at fluid-fluid interfaces or colloids trapped by laser fields. Although this partial confinement allows for motion of the particles only within the plane, their dynamics is influenced by hydrodynamic interactions mediated by the unconfined, three-dimensional flow of the embedding fluid. We demonstrate that this dimensionality mismatch induces a characteristic divergence in the collective diffusion coefficient of the colloidal subsystem. This result, independent of the specific interparticle forces in the monolayer, is solely due to the kinematical constraint on the colloidal particles, and it is different from the known divergence of transport coefficients in purely one or two-dimensional fluids. We study the consequences for two different setups: We find anomalous diffusion for an ideal-gas-like system of non-interacting colloidal particles and a significant speedup for the capillary induced collapse of a colloidal patch at a fluid interface.

15 min break

Invited Talk

CPP 17.6 Tue 11:15 ZEU 260

Molecular Dynamics simulations of the glass transition in 1,4-polybutadiene confined by graphite walls — ●WOLFGANG PAUL¹, MATHIEU SOLAR¹, and KURT BINDER² — ¹Institut für Physik, Martin-Luther-Universität, 06099 Halle — ²Institut für Physik, Johannes-Gutenberg-Universität, 55099 Mainz

We will discuss simulations of a chemically realistic representation of 1,4-polybutadiene (PBD) between graphite surfaces and discuss the influence of the walls on structure and dynamics in the polymer film. There have been many studies of polymers at interfaces and especially on the influence of interfaces on the glass transition in polymers, and with partially contradicting results. We will show that there are two influences of the wall on the structure in the adjacent melt. The first is a strong layering in the monomer density next to the wall, and the second is an orientation of the chains close to the wall and a layering in the centre of mass density of the chains.

Both structural effects give rise to significant modifications of the relaxation behaviour of the polymer next to the wall. We will discuss in detail how these can be identified in different experiments ranging from dielectric spectroscopy to nuclear magnetic resonance to neutron scattering. Determining the glass transition temperature of the confined system from the dielectric relaxation, we find that for this realistic polymer wall model it is independent of the thickness of the film studied down to about 1 nm.

CPP 17.7 Tue 11:45 ZEU 260

Enhanced Dispersion by Elastic Turbulent Flow Through Porous Media — ●CHRISTIAN SCHOLZ¹, FRANK WIRNER¹, and CLEMENS BECHINGER^{1,2} — ¹Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — ²Max-Planck-Institut für Intelligente Systeme, Heisenbergstraße 3, 70569 Stuttgart, Germany

We experimentally investigate hydrodynamic dispersion of micron-

sized tracer particles in elastic turbulent flows of semi-dilute polymer solutions through a periodic porous medium at ultra low Reynolds numbers $Re < 5 \times 10^{-4}$. The asymptotic behaviour of the transversal mean squared displacement is linear and characterized by a dispersion coefficient D_{\perp} , that grows non-linearly with the Weissenberg number Wi and is several orders of magnitude larger compared to laminar flow. While the enhanced velocity fluctuations appear as Wi dependent noise, for Wi far away from the onset of elastic turbulence we observe a non-linear asymmetry in the flow field.

CPP 17.8 Tue 12:00 ZEU 260

Hydrodynamic dispersion of micron-sized colloids in micro-structured porous media — ●FRANK WIRNER¹, CHRISTIAN SCHOLZ¹, and CLEMENS BECHINGER^{1,2} — ¹Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — ²Max-Planck-Institut für Intelligente Systeme, Heisenbergstraße 3, 70569 Stuttgart, Germany

The flow of liquids through porous media is of importance in many areas, such as groundwater pollution, secondary oil recovery or blood perfusion inside the body. The complex geometry of porous media can give rise to a combination of principal pathways, along which particles are transported by advection, and stagnant parts, wherein particles can only move slowly by diffusion. Especially in porous media with low porosities these stagnant parts may eventually dominate the transport properties of fluids and colloids. The mean sojourn time of a particle in a stagnant part, however, can easily exceed experimentally accessible time scales. Therefore, we investigate the effect of stagnant parts on the transit times of micron-sized particles in quasi-two-dimensional porous structures by a semi-experimental approach, which enables us to capture these rare events. The longest transit times can be related to the stagnant parts of the structure, whereby it might be possible to predict the amount of trapped fluid in porous media.

CPP 17.9 Tue 12:15 ZEU 260

Single water molecule confined in a nano-cavity of beryl crystal lattice — ●MARTIN DRESSEL¹, E.S. ZHUKOVA^{1,2,3}, V.I. TORRASHEV⁴, V.V. LEBEDEV^{3,5}, G.S. SHAKUROV⁶, R.K. KREMER⁷, E.V. PESTRJKOV⁸, V.G. THOMAS⁹, D.A. FURSENKO⁹, and B.P. GORSHUNOV^{1,2,3} — ¹Phys. Inst., Univ. Stuttgart — ²A.M. Prokhorov Gen. Phys. Inst., RAS, Moscow — ³Moscow Inst. Phys. Techn., Dolgoprudny — ⁴Fac. Phys., Southern Fed. Univ. Rostov-on-Don — ⁵Landau Inst. Theor. Phys., RAS, Chernogolovka — ⁶Kazan Phys.-Techn. Inst., RAS, Kazan — ⁷MPI Festkörperforschung, Stuttgart — ⁸Inst. Laser Phys., RAS, Novosibirsk — ⁹Inst. Geology Mineralogy, RAS, Novosibirsk

Using terahertz and infrared spectroscopy, we have studied the low-energy excitations of a single H₂O molecule confined within a nano-cage formed by ions of beryl (Mn:Be₃Al₂Si₆O₁₈) crystal lattice. At terahertz frequencies, for electric field of the probing radiation polarized perpendicular to the crystallographic *c*-axis ($E \perp c$) multiple resonances are discovered and assigned to librational and translational vibrations of the H₂O molecule that is weakly (via hydrogen bonds) coupled to the walls of the nano-cage. Only two water-related absorption peaks are seen for the second polarization $E \parallel c$. A model is presented that explains the resonances by taking into account the quantum tunneling between the H₂O states in the minima of a six-well potential felt by a molecule within the cage. We draw analogies with the electrodynamic spectra of liquid water and ice.

Ref.: B.P. Gorshunov et al., J. Phys. Chem. Lett. 4, 2015 (2013).

CPP 17.10 Tue 12:30 ZEU 260

Gold Nano-Structure Assisted Thermophoretic Trapping of Single Nano-Objects — ●MARCO BRAUN and FRANK CICHOS — Molecular Nanophotonics, Fakultät für Physik und Geowissenschaften Universität Leipzig, Deutschland

Single molecule spectroscopy has become indispensable in today's soft-matter sciences. Brownian motion scaling with the molecules hydrodynamic radius lets it quickly disappear from the observation volume, which is why the molecule of interest is typically immobilized in a polymer matrix or by chemical interactions, generally accepted due to a lack of alternatives. Here, we present an all-optical technique to trap single nano-objects in solution which exploits 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 induces a particle drift. In our approach the temperature field is generated by an optically heated gold nano-structure. 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 Brownian particles can be manipulated.

In our experiment an appropriate gold structure is heated locally by a focused laser beam with feedback to the Brownian particles position.

CPP 18: Wetting, Superamphiphobicity, Micro- and Nanofluidics I

Time: Tuesday 9:30–12:45

Location: ZEU 222

CPP 18.1 Tue 9:30 ZEU 222

A liquid-vapor interface at equilibrium in the vicinity of structured substrates: a mean-field approach — ●NIKITA TRETAYAKOV, BURKHARD DÜNNEWEG, and KOSTAS DAOULAS — Max Planck Institute for Polymer Research, Mainz, Germany

We study static properties of a liquid-vapor interface in the vicinity of structured substrates employing a mean-field approach [1]. As opposed to the particle-based simulations [2], this is a continuum method based on thermodynamics and statistical physics. To this end, the Hamiltonian of the system is written to account for the bulk phases, the interface [3] and the interaction with the solid. The model is then proved by a series of case-studies. Later on, we use different geometries of the substrate to investigate the interface' response to external pressure and support our simulations with analytical results.

[1] K. M. Hong and J. Noolandi, "Theory of inhomogeneous multicomponent polymer systems", *Macromolecules*, vol. 14, no. 3, pp. 727-736, 1981.

[2] N. Tretayakov and M. Müller, "Correlation between surface topography and slippage: a molecular dynamics study", *Soft Matter*, vol. 9, pp. 3613-3623, 2013.

[3] K. R. Mecke and S. Dietrich, "Effective hamiltonian for liquid-vapor interfaces", *Phys. Rev. E*, vol. 59, pp. 6766-6784, 1999.

CPP 18.2 Tue 9:45 ZEU 222

Understanding the effect of temperature on hydrophobic wetting through molecular dynamics simulations — ●FRÉDÉRIC LEROY — Technische Universität Darmstadt, Darmstadt, Germany

Hydrophobic surfaces usually yield water contact angles which weakly depend on temperature. To explain this observation, we address the thermodynamics of formation of interfaces between rigid non-polar solid surfaces and water. The work of adhesion of water can be separated in its enthalpy and entropy contributions per unit area $W = \Delta H / A - T \Delta S / A$. [1] While the enthalpy relates to the energy loss upon separating the liquid and the solid phases, the entropy change characterizes the entropy gain of water upon separation. Inspired by the analogy between the solvation of particles in water and the formation of solid-liquid contacts, a clear microscopic interpretation of both contributions in terms of intermolecular interaction potentials is given. [2] We illustrate how the determination of ΔH and ΔS by means of molecular simulations of water on rigid non-polar surfaces explains why the work of adhesion has a greater temperature dependence on hydrophobic than on hydrophilic surfaces. [3,4]

[1] Taherian, F.; Marcon, V.; van der Vegt, N.F.A and Leroy, F. "What is the Contact Angle of Water on Graphene?" *Langmuir* 29, 1457-1465 (2013) [2] Taherian, F.; Leroy, F and van der Vegt, N.F.A. "Interfacial Entropy of Water on Rigid Hydrophobic Surfaces" *Langmuir* 29, 9807-9813 (2013) [3] Kumar, V. and Errington, J.R. "Wetting Behavior of Water near Nonpolar Surfaces", *J. Phys. Chem. C* 117, 23017-23026 (2013) [4] Leroy, F., in preparation

CPP 18.3 Tue 10:00 ZEU 222

Liquid drops on a surface: using density functional theory to calculate the binding potential and drop profiles and comparing with results from mesoscopic modelling — ●ADAM P. HUGHES¹, UWE THIELE^{1,2}, and ANDREW J. ARCHER¹ — ¹Department of Mathematical Sciences, Loughborough University, UK — ²Institut für Theoretische Physik, Universität Münster, Germany

The contribution to the excess free energy for a film of liquid of thickness h on a solid surface, due to the interactions between the solid-liquid and liquid-gas interfaces is given by the binding potential, $W(h)$. The precise form of $W(h)$ determines whether or not the liquid wets the surface. Note that differentiating $W(h)$ gives the Derjaguin or disjoining pressure. We develop a microscopic density functional theory (DFT) based method for calculating $W(h)$, allowing us to relate the form of $W(h)$ to the nature of the molecular interactions in the system. We present results using a simple lattice gas model to demonstrate the

procedure. In order to describe non-uniform liquid films and drops, a mesoscopic free energy based on $W(h)$ is often used. We calculate such film height profiles and also directly calculate using DFT the corresponding density profiles for liquid drops on surfaces. Comparing quantities such as the contact angle and also the shape of the drops, we find good agreement between the two methods. We also study in detail the effect on $W(h)$ of truncating the range of the dispersion forces, both those between the fluid molecules and those between the fluid and wall. We find that truncating can have a significant effect on $W(h)$ and the associated wetting behaviour of the fluid.

CPP 18.4 Tue 10:15 ZEU 222

Droplet morphologies upon volume change on structured substrates — ●CARSTEN HERRMANN¹, CIRO SEMPREBON², MARTIN BRINKMANN^{1,2}, and RALF SEEMANN^{1,2} — ¹Saarland University, 66041 Saarbrücken — ²Max Planck Institute for Dynamics and Self-Organization, 37018 Göttingen

We experimentally investigate the general behavior of droplet morphologies sitting on micro-structured substrates upon volume change. The substrates provide geometries like triangular, rectangular, sinusoidal and trapezoidal cross section. 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. The morphological changes depend sensitively on the wettability, aspect ratio and geometry of the underlying grooved substrate. The experimental results are compared quantitatively with numerical results computed by minimizing surface energies

CPP 18.5 Tue 10:30 ZEU 222

How superhydrophobicity breaks down — ●PERIKLIS PAPAPOPOULOS, FRANK SCHELLENBERGER, LENA MAMMEN, XU DENG, DORIS VOLLMER, and HANS-JÜRGEN BUTT — Max Planck Institute for Polymer Research, D-55128 Mainz, Germany

Droplets on superhydrophobic surfaces roll off easily, leaving the surface dry and clean. This property is due to a surface geometry that favors the entrainment of air beneath the drop, leading to the so-called Cassie state. This state competes with the Wenzel (impaled) state, in which the liquid fully wets the substrate. Despite the fact that thermodynamically the Wenzel state is often more stable, the geometry imposes an energy barrier that prevents the liquid from wetting the structure. The transition dynamics is still poorly understood due to difficulties in monitoring the temporal evolution of the liquid-air meniscus between the asperities with sufficient spatial resolution. Here, we study the Cassie-to-Wenzel transition of water drops evaporating on arrays of hydrophobic micropillars. To understand the underlying processes, we image the impalement dynamics in three dimensions by confocal microscopy. As evaporation proceeds, the curvature of the drop and the Laplace pressure increase. The three-phase contact line remains pinned until the contact angle reaches the advancing contact angle of the material. Then the water slides down the pillars. Alternatively, at large pillar spacing the curved water surface can touch the bottom of the substrate triggering an instantaneous Cassie-to-Wenzel transition. [1] Papadopoulos P., Mammen L., Deng X., Vollmer D., Butt H.-J., *PNAS* 110, 3254-3258 (2013)

CPP 18.6 Tue 10:45 ZEU 222

Superamphiphobic particles - how small can we go? — MING YE, XU DENG, JAVED ALLY, PERIKLIS PAPAPOPOULOS, FRANK SCHELLENBERGER, DORIS VOLLMER, MICHAEL KAPPL, and ●HANS-JÜRGEN BUTT — Max-Planck-Institut für Polymerforschung, Mainz, Germany

Water and oil repellent coatings - so called superamphiphobic coatings - greatly reduce the interaction between a liquid and a solid. So far only flat or weakly curved superhydrophobic and superamphiphobic surfaces have been designed. This raises the question whether highly curved structures or microspheres are feasible.

Therefore, we coated microspheres with a superamphiphobic layer and measured the force between the spheres and a liquid. A qualitatively different dependence of the adhesion force on the applied load for superamphiphobic and smooth spheres is detected. Furthermore we demonstrate both experimentally and theoretically that superamphiphobicity fails below a critical particle radius, depending on topological details and type of liquid. Therefore, this study sets a fundamental physical limit to the application of superamphiphobic layers for small objects with high curvature.

15 min. break

CPP 18.7 Tue 11:15 ZEU 222

Gibbs condition for a volatile completely wetting liquid — ●MARIANO GALVAGNO¹, IOANNIS TSOUMPAS², PIERRE COLINET², and UWE THIELE^{1,3} — ¹Department of Mathematical Sciences, Loughborough University, UK — ²TIPs-Fluid Physics, Université Libre de Bruxelles, Belgium — ³Institut für Theoretische Physik, Universität Münster, Germany

We study the profile of evaporating liquid drops on substrates with a corner. A continuous influx allows us to study steady drops of different volume even in this non-equilibrium situation. Experimental results are qualitatively reproduced employing a 2d long-wave mesoscopic hydrodynamic description that incorporates wettability via a Derjaguin (disjoining) pressure. In particular, we study (i) the dependence of the evaporation-induced apparent contact angle on the position of the contact line and (ii) the pinning and depinning of a droplet at a corner - that is for non-volatile liquids well described by Gibbs' criterion. Our results suggest that for volatile liquids, a simple modification of Gibbs' criterion is valid: replacing the equilibrium contact angle by the evaporation-caused apparent contact angle. Most importantly, the calculations confirm the experimental observation, that there exists a dynamically produced critical angle for depinning that increases with the evaporation rate.

CPP 18.8 Tue 11:30 ZEU 222

Slip effects in dewetting polymer microdroplets — ●JOSHUA D. MCGRAW¹, THOMAS SALEZ², SIMON MAURER¹, TAK SHING CHAN^{1,3}, MICHAEL BENZAQUEN², JONAS HEPPE¹, MARTIN BRINKMANN^{1,3}, ÉLIE RAPHAËL², and KARIN JACOBS¹ — ¹Saarland University, Experimental Physics, D-66041 Saarbrücken — ²Laboratoire de Physico-Chimie Théorique, UMR CNRS Gulliver 7083, ESPCI, Paris, France — ³Max Planck Institute for Dynamics & Self-Organization, 37077 Göttingen

Spherical caps on a substrate with less than equilibrium contact angles contract as a result of capillary forces. Applying the classical no-slip condition at the liquid-substrate interface results in diverging stress at the contact line. This divergence can be alleviated, however, by allowing finite flow velocity at the substrate, corresponding to the slip boundary condition. Experiments have been conducted in which glassy polystyrene microdroplets are placed upon, as substrates, different self-assembled monolayers (SAMs). The spherical caps are prepared such that initial contact angles are much less than the equilibrium contact angle. Above the glass transition temperature, a capillary induced flow is observed; the droplet radii shrink while their heights grow. Furthermore, the intermediate height profiles are highly non-spherical. Different SAMs give rise to differing slip lengths, resulting in dramatic changes to the temporal and morphological path these tiny droplets take toward their equilibrium spherical cap shapes.

CPP 18.9 Tue 11:45 ZEU 222

Wetting and electrowetting — MARKUS BIER and ●INGRID IBAGON — MPI for Intelligent Systems, Stuttgart, Germany

The phenomenon of electrowetting, i.e., the dependence of the macroscopic contact angle of a fluid on the electrostatic potential of the substrate, is analyzed in terms of the density functional theory of wetting. A comparison with the traditional scheme based on capacitor models reveals qualitative errors of the latter approach. Within density functional theory one accounts for the formation of a microscopically thin film which (partially) wets the substrate. By that means one obtains an improved expression for the electrowetting number as a function of

the voltage. The improved theory is compared with available experimental results and with predictions of the traditional approach. An experimental setup is proposed to differentiate between the traditional and the density functional approach to electrowetting.

CPP 18.10 Tue 12:00 ZEU 222

Liquid transport on rough substrates — CIRO SEMPREBON, ●STEPHAN HERMINGHAUS, and MARTIN BRINKMANN — MPI-DS Goettingen

The ability of liquids to form continuous films on solids is essential for many technical applications such as surface coatings or liquid transport in granulates. In this work we investigate the morphological evolution and transport properties of wetting layers adhering to an irregular rough substrate. To avoid explicit modelling of contact lines, we consider a thin film model with a precursor film and minimize the total interfacial energy. The generic short range interface potential accounts for a finite apparent contact angle of the macroscopically thick regions of the film. Based on the static interfacial profiles obtained by energy minimization, we numerically solve the linearized steady thin film equation and compute the effective mobility of the liquid. Various types of roughness and material contact angles are investigated, either prescribing the pressure in or the volume of the liquid film. Our results show that the connectivity between the domains of macroscopically thick films can be correlated to the effective liquid mobility.

CPP 18.11 Tue 12:15 ZEU 222

Forced multiphase flow on the pore scale explored in 3D — ●HAGEN SCHOLL¹, KAMALJIT SINGH², ALEN KABDENOV¹, MARIO SCHEEL², and STEPHAN HERMINGHAUS³ — ¹Saarland University, Saarbrücken, Germany — ²ESRF, Grenoble, France — ³MPI-DS, Göttingen, Germany

Using ultra fast x-ray tomography the forced imbibition of an aqueous phase into an initially oil filled matrix is studied. The water is volume controlled flushed into cylindrical columns filled with oil saturated spherical bead packs and the forced imbibition is imaged in real time using ultrafast x-ray tomography. The 3d time series are analyzed in terms of oil content, front area and the pore throat filling behavior. For typical flow parameter at low capillary numbers, as e.g. relevant for oil recover, the multiphase flow hardly depends on gravitational effects and details of the pore space. Capillary forces, however, are a key to understand the forced multiphase flow. A compact front develops for a wettable invading phase whereas a branched front develops for a non-wettable invading phase.

CPP 18.12 Tue 12:30 ZEU 222

Adsorption kinetics of surfactants in droplet-based microfluidics using pH measurements at the micron scale — ●BIRTE RIECHERS, QUENTIN BROSSEAU, FLORINE MAES, and JEAN-CHRISTOPHE BARET — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Interfaces are omnipresent in biological and man-made systems like emulsions and foams. In biology, interfaces are particularly important for encapsulation and compartmentalization [Theberge et al. *Angewandte* 2010]. They can be stabilized using surfactants which, upon adsorption, influence properties of the interface (e.g. surface tension and interfacial rheology) and of the bulk phases (e.g. pH) [Baret *LabChip* 2012]. The determination of interfacial properties (equilibrium, adsorption kinetics to the interface) at the scale of the emulsion droplets is crucial for their use in biotechnological applications and solves a fundamental problem.

We present a new method for the determination of the dynamics of surfactant adsorption and surfactant coverage at the interface using droplet-based microfluidics. Water-in-oil emulsions are studied using a fluorescence setup. In combination with a pH sensitive dye inside the droplets, adsorption kinetics of an acidic surfactant are monitored. As the surfactant adsorbs to the interface and deprotonates, it changes the pH inside the dispersed phase giving rise to adsorption and equilibrium properties. We show the effectiveness of surfactant adsorption in droplet-based microfluidics and unravel the kinetics of adsorption at the micron scale with a millisecond time-resolution.

CPP 19: Poster Session 1 (joint session with BP)

Organic Electronics and Photovoltaics, Biomaterials and Biopolymers, Ionic Liquids, Glasses

Time: Tuesday 9:30–13:00

Location: P1

CPP 19.1 Tue 9:30 P1

The solid-liquid interface of ionic liquid solutions – Interfacial layering and solvent-induced screening — ●MARKUS MEZGER^{1,4}, HEIKO SCHRÖDER¹, PETER REICHERT^{1,4}, ROLAND ROTH², HARALD REICHERT³, and DIEGO PONTONI³ — ¹Max-Planck-Institut für Polymerforschung, 55128 Mainz, Germany — ²Eberhard Karls Universität, 72076 Tübingen, Germany — ³European Synchrotron Radiation Facility, 38043 Grenoble, France — ⁴Johannes Gutenberg Universität, 55128 Mainz, Germany

The influence of the polar, aprotic solvent propylene carbonate on the interfacial structure of the ionic liquid 1-butyl-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphat ([bmpy⁺][FAP⁻]) on sapphire was investigated by high-energy x-ray reflectivity. Analysis of our experimental data revealed interfacial profiles comprised of alternating anion and cation enriched regions decaying gradually into the bulk liquid. With increasing solvent concentration, a decrease in the decay length of the interfacial layering structure was observed. Solvent molecules were found to accumulate laterally within the layers, hence screening the charges between like ions. The results are compared with the bulk structure of IL-solvent mixtures.

CPP 19.2 Tue 9:30 P1

Molecular Scale Structure of Ionic Liquid-Aqueous Solution Interfaces — ●XILIN WU¹, JULIAN MARS¹, BINYANG HOU^{1,2}, VEIJO HONKIMÄKI², and MARKUS MEZGER^{1,3} — ¹Max-Planck-Institut für Polymerforschung, 55128 Mainz, Germany — ²European Synchrotron Radiation Facility, 38043 Grenoble, France — ³Johannes Gutenberg-Universität, 55128 Mainz, Germany

Ionic liquids (ILs) are widely used as environmental friendly solvents for liquid-liquid extraction processes. However only little is known on their molecular scale structure near fluid interfaces. We employed high energy x-ray reflectivity (XRR) to study the free surface and the buried IL-water interface of 1-butyl-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphat ([bmpy⁺][FAP⁻]). The influence of metal cations on the interfacial structure was probed by adding cobalt ions ([Co²⁺][Cl₂⁻]) to the aqueous phase. The Electron density profile across the IL-aqueous solution interface was extracted from the experimental XRR data. Its dependence on the interfacial potential was studied by time-resolved XRR measurements recorded during cyclic voltammetry. The data shows clear correlations between the applied voltage and the XRR intensity, indicating potential induced ion rearrangement at the liquid-liquid interface.

CPP 19.3 Tue 9:30 P1

Photoelectron Spectroscopy on Ionic Liquid Surfaces – Theory and Experiment — ●WICHARD J. D. BEENKEN¹, ANGELA ULBRICH¹, MARKUS REINMÖLLER², and STEFAN KRISCHOK¹ — ¹Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany — ²TU Bergakademie Freiberg, Institut für Energieverfahrenstechnik und Chemieingenieurwesen, Freiberg, Germany

We have studied various ionic liquids by photoemission spectroscopy. For a more in depth interpretation of the experimental results, in particular of valence spectra, a theoretical reconstruction of these spectra by means of density functional theory is desired. In order to obtain correct binding energies and peak intensities a simple calculation of the density of states is not sufficient. A self-developed method, which bases on known elementary cross sections for the photoeffect and adjustments of the kinetic energy of emitted electrons is applied. Particular attention is paid to the necessary relative shift for cation and anion due to their different Madelung potentials. In order to study this effect, we have varied the cations and the anions of the ionic liquids under investigation, systematically.

CPP 19.4 Tue 9:30 P1

Influence of cation on lithium transport in ionic liquid/Li-salt electrolyte: A molecular dynamics study — ●VOLKER LESCH¹, ANDREAS HEUER¹, ZHE LI², and DMITRY BEDROV² — ¹Westfälische Wilhelms-Universität Münster — ²University of Utah

Molecular Dynamics (MD) simulations is a powerful tool to get atomic scale understanding of different systems. Room temperature ionic li-

uids have been considered as new alternative materials for variety of applications, including as electrolytes for Li-ion batteries and supercapacitors. Addition of lithium salt to an ionic liquid results in strong interactions between anions with the small lithium ion and significantly alters electrolyte properties. However the details of the chemical structure of the ionic liquid cation and its influence on the lithium ion coordination and overall electrolyte properties are not well understood. Here we compare MD simulations of ionic liquids comprised of 1-Ethyl-3-methylimidazolium or N-methyl-N-propylpyrrolidinium cations paired with tri-(bis-fluorosulfonyl)-imide (TFSI) anion and mixed with LiTFSI salt. We performed MD-simulations of both ionic liquids with lithium salts at different temperatures and salt concentrations and examined the influence of cation properties (chemical structure, size, charge distribution) on electrolyte transport properties such as self-diffusion coefficients, ionic conductivity, and viscosity. These transport properties and the mechanisms of Li ion mobility were correlated with Li-ion local coordination structure and anion exchange rates inside the Li-ion first coordination shell.

CPP 19.5 Tue 9:30 P1

Layer Formation of Alkylimidazolium Ionic Liquids at the Sapphire/Liquid Interface — ●MICHAEL KLIMCZAK¹, NICOLA TACCARDI², and ANDREAS MAGERL¹ — ¹Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen-Nürnberg — ²Lehrstuhl für Chemische Reaktionstechnik, Universität Erlangen-Nürnberg

Alkylimidazolium-based room temperature ionic liquids (RTILs) – among others – are known to form well-ordered structures in contact with smooth metal or oxide interfaces [1]. By means of specular X-ray reflectivity (XRR) interface normal electron density profiles are obtained with submolecular resolution giving detailed insight of structures at the interface [2]. 1-ethyl-3-methylimidazolium-bis(trifluoromethylsulfonyl)imide [EMIM][NTf₂] is shown to form a stack of alternating cation/anion monolayers at the (0001) sapphire/liquid interface. The first layer is confirmed to be composed of cations with their imidazolium rings parallel to the interface, followed by about five clearly distinguishable double layers.

With longer alkyl chains – replacing [EMIM] cations by [HMIM] (1-Hexyl-3-Methylimidazolium) or [DMIM] (1-Decyl-3-Methylimidazolium) – alternating cation/anion structures are still observed with the length and orientation of the alkyl chains significantly influencing the layering properties.

[1] H. Li, F. Endres, and R. Atkin, *Physical Chemistry Chemical Physics*: PCCP 15, 14624 (2013).

[2] M. Mezger, H. Schröder, and H. Reichert, *Science* 322, 424 (2008).

CPP 19.6 Tue 9:30 P1

New method for volatility determination of ionic liquids at the nanoscale by means of ultra-fast scanning calorimetry — ●MATHIAS AHRENBERG¹, MARCEL BRINCKMANN¹, JÜRGEN W.P. SCHMELZER¹, MARTIN BECK², CHRISTIN SCHMIDT³, OLAF KESSLER², UDO KRAGL³, SERGEY P. VEREVKIN³, and CHRISTOPH SCHICK¹ — ¹Institute of Physics, University of Rostock, Wismarsche Str. 43-45, 18051 Rostock, Germany — ²Faculty of Mechanical Engineering and Marine Technology, University of Rostock, Albert-Einstein-Str. 2, 18059 Rostock, Germany — ³Institute of Chemistry, University of Rostock, Albert-Einstein-Str. 3a, 18059 Rostock, Germany

Here we present a new method for the determination of vaporization enthalpies of Ionic Liquids using differential fast scanning calorimetry. We have developed and proven this method using [EMIm][NTf₂] at temperatures up to 750 K and in different atmospheres. This method allows very high heating rates (up to 100000 K/s) and thus much higher temperatures can be reached in the measurement of the mass loss rate as compared to common devices without significant decomposition of the ionic liquid.

CPP 19.7 Tue 9:30 P1

Polymeric nanoparticles for drug delivery, stability and pH response — ●NATALYA VISHNEVETSKAYA¹, MARGARITA DYAKONOVA¹, ANNA BOGOMOLOVA², SERGEY FILIPPOV², and CHRISTINE PAPADAKIS¹ — ¹TU München, Physikdepartment, Physik weicher Materie — ²Institute of Macromolecular Chemistry, Prague, Czech Republic

Polymer-drug conjugates based on the copolymer N-(2-hydroxypropyl) methacrylamide (HPMA) bearing the anticancer drug doxorubicin and a defined amount of hydrophobic moieties (cholesterol and its derivatives) are therapeutically highly potent. The structures of the pH cleavable cholesterol-HPMA linkage and of cholesterol itself influence on the nanoparticle formation and behavior in solution [1].

The micelle formation of various copolymers in phosphate buffer solution and their size was investigated using fluorescence correlation spectroscopy (FCS) by adding the fluorescence dye rhodamine 6G. We have compared the values of the hydrodynamic radii of the micelles and the critical micelle concentrations in very dilute solutions (as in blood) of the copolymers as well as the kinetics during time and pH changes. Using dynamic light scattering, the average size of the nanoparticles and their stability in various environments are studied, and (time-resolved) small-angle neutron scattering provides detailed information on the micellar core-shell structures.

[1] S.K. Filippov et al., *Biomacromolecules* 14, 4061 (2013)

CPP 19.8 Tue 9:30 P1

Energetics, optical response and spin structure of μ - η^2 : η^2 -peroxo and bis- μ -oxo dicopper model complexes calculated within (TD)DFT and MBPT — ●MARTIN ROHRMÜLLER¹, SONJA HERRES-PAWLIS², and WOLF GERO SCHMIDT¹ — ¹Theoretische Physik, Universität Paderborn, 33098 Paderborn, Germany — ²Department Chemie, Ludwig-Maximilians-Universität München, 81377 München, Germany

Binuclear Cu complexes play an important role in the enzymatic oxidation and are of potential interest for industrial redox processes [1]. However, the physics and chemistry of the corresponding charge transfer mechanism are not yet fully understood. In order to contribute to a microscopic understanding of the charge and structural dynamics in such complexes we focus on the characterisation of the transition of model systems from bis- μ -oxodicopper(III) species (O) to μ - η^2 : η^2 -peroxodicopper(II) species (P).

We investigate ground-state as well as excited-state potential energy surfaces, with particular emphasis on the influence of the spin structure. Optical response and electronic excitations are calculated using (Time Dependent) Density Functional Theory and Many Body Perturbation Theory [2]. Based on these findings we use non-adiabatic trajectory surface hopping [3] to tackle the pico second dynamics.

[1] Solomon *et al.*, *Chem. Rev.* 1996, **96**, 2563

[2] M. Rohrmüller *et al.*, *J. Comp. Chem.* 2013, **34**, 1035-1045

[3] M. Barbatti, *WIREs Comput Mole Sci*, 2011, **1**, 620-633

CPP 19.9 Tue 9:30 P1

Femtosecond dynamics of optically excited dicopper complexes — ●ANDREAS LÜCKE, MARTIN ROHRMÜLLER, and WOLF GERO SCHMIDT — Universität Paderborn, Lehrstuhl für Theoretische Physik, Germany

Copper proteins are of particular interest as they are crucial for biological functions like oxygen transport or cellular respiration [1]. Here we focus on bis-(μ -oxo)dicopper model complexes that contain a $[Cu_2O_2]^{2+}$ core. By means of comparison to results of many-body perturbation theory, i.e. quasiparticle calculations within the GW approximation and subsequent solution of the Bethe-Salpeter equation, it is shown that time-dependent density-functional theory (TDDFT) within the adiabatic approximation reliably describes the molecular optical response of the molecules [2]. Based on this finding, real-time TDDFT is used to explore the molecular electron dynamics in response to the optical excitation. Thereby the time-dependent Kohn Sham equations are solved to describe the electron relaxation on the femtosecond timescale.

[1] E. A. Lewis and W. B. Tolman, *Chem. Rev.* 2004, 104, 1047-1076

[2] M. Rohrmüller, S. Herres-Pawlis, M. Witte, and W. G. Schmidt, *J. Comp. Chem.* 2013, 34, 1035-1045

CPP 19.10 Tue 9:30 P1

Excited state proton transfer reaction pathways: Ab-initio study of solvated 7-Hydroxyquinoline — ●GÜL BEKÇIOĞLU, CHRISTOPH ALLOLIO und DANIEL SEBASTIANI — Institut für Chemie, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 4, 06120 Halle (Saale), Deutschland

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]. Upon excitation, Hy-

droxyquinolones (HQ) are simultaneously photoacids and photobases. We study the ground and excited state solvation of 7HQ, focussing on the identification of water wires and excited state protonation dynamics. Additionally, we characterize a novel pathway which has not been discussed in literature so far, namely the transfer of an anionic hydroxide ion species through a short water wire, initiated by proton donation to the photobasic site of 7HQ.

[1] F. Garczarek and K. Gerwert, *Nature* 439 (2006), 109-112. [2] O. F. Mohammed, D. Pines, J. Dreyer, E. Pines and E. T. J. Nibbering., *Science* 310 (2005), 5745.

CPP 19.11 Tue 9:30 P1

Excited state proton transfer reaction pathways: Ab-initio study of solvated 7-Hydroxyquinoline — ●GÜL BEKÇIOĞLU, CHRISTOPH ALLOLIO und DANIEL SEBASTIANI — Institut für Chemie, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 4, 06120 Halle (Saale), Deutschland

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]. Upon excitation, Hydroxyquinolones (HQ) are simultaneously photoacids and photobases. We study the ground and excited state solvation of 7HQ, focussing on the identification of water wires and excited state protonation dynamics. Additionally, we characterize a novel pathway which has not been discussed in literature so far, namely the transfer of an anionic hydroxide ion species through a short water wire, initiated by proton donation to the photobasic site of 7HQ.

[1] F. Garczarek and K. Gerwert, *Nature* 439 (2006), 109-112.

[2] O. F. Mohammed, D. Pines, J. Dreyer, E. Pines and E. T. J. Nibbering., *Science* 310 (2005), 5745.

CPP 19.12 Tue 9:30 P1

FTIR-spectroscopy reveals the pressure-dependent interplay between internal and external constraints in spider silk — ●ARTHUR MARKUS ANTON¹, ROXANA FIGULI², PERIKLIS PAPADOPOULOS³, and FRIEDRICH KREMER¹ — ¹Institut für Experimentelle Physik I, Universität Leipzig, Germany — ²Institut für Technische Chemie und Polymerchemie, Karlsruher Institut für Technologie, Germany — ³Max Planck Institut für Polymerforschung, Germany

Due to its unique mechanical properties, namely high tensile strength combined with great elasticity, spider silk surpasses modern synthetic fibers [S. Kubik, *Angew. Chem. Int. Ed.* **41** (2002)]. Until recently, one was incapable of manufacturing materials with similar properties on a large scale [M. Heim et al., *Angew. Chem. Int. Ed.* **48** (2009)], because of an incomplete understanding of spider silk's microscopic structure. Its mechanical properties are based on a refined architecture at the molecular and mesoscopic scale. β -sheet nanocrystals are interconnected through *prestrained* amorphous regions offering an internal force counterbalanced by the fiber's outer skin. Due to that structure, external stress is directly transferred to the nanocrystals evident in a shift of an Alanine-specific IR absorption band [P. Papadopoulos et al., *Eur. Phys. J. E* **24** (2007); R. Ene et al., *Soft Matter* **5** (2009)]. To unravel this interplay between internal and external constraints a pressure-dependent analysis of this Alanine-specific band by means of hydrostatic pressure provided by a diamond anvil cell (DAC) was carried out [A. M. Anton et al., *Macromol.* **46** (2013)].

CPP 19.13 Tue 9:30 P1

Bundling of grafted, reversibly crosslinked biopolymers — ●DANIEL WILKIN, RICHARD VINK, and ANNETTE ZIPPELIUS — Institute for Theoretical Physics, Georg-August University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

In this poster, we present a Monte Carlo simulation of a system consisting of parallel aligned polymers which are grafted perpendicularly on a flat surface. The polymers are described as weakly-bending chains (persistence length much larger than the polymer length) and neighboring chains can be reversibly crosslinked (the crosslinks being modeled as harmonic springs which induces an attractive force between the polymers). Upon increasing the number of crosslinks, our simulations reveal a transition from a homogeneous state to a state where the polymers have grouped themselves into bundles. When the polymers are grafted on the surface randomly, the bundles appear to be frozen in space (i.e. once they have formed, they never dissolve). In contrast, by grafting the polymers regularly on a lattice, the resulting bundles are mobile, i.e. they form and disappear again at any spatial location

on the surface.

CPP 19.14 Tue 9:30 P1

Mapping nanomechanical properties of hydrated type-I collagen fibrils with MUSIC mode AFM — JULIA HANN¹, DIANA VOIGT¹, EIKE-CHRISTIAN SPITZNER¹, ANKE BERNSTEIN², and ROBERT MAGERLE¹ — ¹Chemische Physik, Fakultät für Naturwissenschaften, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — ²Muskuloskelettales Forschungslabor, Department Orthopädie und Traumatologie, Universitätsklinikum Freiburg, Freiburg i. Br., Germany

Type-I collagen forms fibrils with water embedded between the tropocollagen molecules. The amount and distribution of structural, free, and adsorbed water has a large impact on the fibril's mechanical properties. We study native type-I collagen fibrils using multi-setpoint intermittent contact (MUSIC) mode atomic force microscopy (AFM) in air and in phosphate buffered saline (PBS) solution with different salt concentrations. MUSIC mode AFM is based on point-wise recording amplitude and phase of an oscillating AFM cantilever as the tip-sample distance is reduced. In this way, the unperturbed surface, the tip indentation as well as a quantitative and depth-resolved information about the tip-sample interaction is obtained. Our measurements aim at a better understanding of the tip-sample interaction in liquids as well as the structural and nanomechanical properties of native collagen fibrils under physiological conditions. We find that the fibril's shape and its nanomechanical properties in PBS solution differ distinctly from the fibril's properties in air and we discuss the physical origin of these differences.

CPP 19.15 Tue 9:30 P1

Multivalency in the binding of the viral transmembrane protein hemagglutinin with the cellular receptor sialic acid studied by single molecule force spectroscopy — VALENTIN REITER¹, SUMATI BHATIA², MANUEL GENSLER¹, CHRISTIAN SIEBEN¹, DANIEL LAUSTER¹, SUSANNE LIESE², ANDREAS HERRMANN¹, RAINER HAAG², ROLAND NETZ², and JÜRGEN P. RABE¹ — ¹Humboldt-Universität zu Berlin — ²Freie Universität Berlin

We use force spectroscopy techniques based on the scanning force microscope (SFM) to gain insight into the multivalent interactions between the viral transmembrane protein hemagglutinin (HA) and sialic acid (SA), a part of the cellular glyco-proteins. The binding of a virion to its host in order to induce the endocytosis is the first step in the reproduction of the virus and therefore the inhibition of this attachment is a good approach to prevent infection of cells. Custom designed nano particles outfitted with SA can be used as decoy particles to prevent the virion from attaching itself to a cell membrane [1],[2]. In order to increase the probability and efficiency of the binding of the nano particle to the virus the process of binding and unbinding of the HA to the SA has to be well understood, so that scaffolds suitable to fit the HA binding pockets can be designed. In order to obtain insight into the binding affinities, single molecule force spectroscopy (SMFS) can be used by functionalizing the SFM cantilever with receptor molecules and creating structured arrays of the ligand HA using poly histidine tags. [1] I. Papp et al., *small* 2010, 6, No. 24, 2900-2906; [2] I. Papp et al., *ChemBioChem* 2011, 12, 887-895;

CPP 19.16 Tue 9:30 P1

Amino Acid-Sequence Dependent Interactions between Receptors and Ligands Studied with Optical Tweezers — TIM STANGNER¹, CAROLIN WAGNER¹, DAVID SINGER², STEFANO ANGIOLETTI-UBERTI³, CHRISTOF GUTSCHE¹, JOACHIM DZUBIELLA³, RALF HOFFMANN², and FRIEDRICH KREMER¹ — ¹University of Leipzig, Department of Experimental Physics I, D-04103 Leipzig, Germany — ²University of Leipzig, BBZ, D-04103 Leipzig, Germany — ³Humboldt University Berlin, Department of Physics, Berlin 12489, Germany

For diagnostic procedures that rely on monoclonal antibodies (mAbs), it is imperative to know whether the antibody recognizes the epitope of its target peptide/protein specific or whether possible cross-reactions to other forms of the protein may occur. In a previous study non-specific interactions of the phosphorylation-specific mAb HPT-101 to tau-peptides with similar epitopes, differing only by a single isolated phosphorylation site, were detected. Based on this result, it is obvious that the specificity of this mAb refers not exclusively to the phosphorylation pattern but also to the amino acid sequence in the tau peptide. Here, we investigate with the help of optical tweezers assisted dynamic force spectroscopy the influence of single amino acids on the binding of mAb HPT-101 to the peptide tau[pThr231/Ser235]. For this purpose,

we characterize the unbinding process by analyzing the measured rupture force distributions. Furthermore, the binding process is specified by means of the relative binding frequency. Using these parameters, it is possible to identify essential as well as secondary amino acids for the interaction of this receptor-ligand system.

CPP 19.17 Tue 9:30 P1

Quantification of DNA Damage by ROS using AFM Tapping Mode — FLORIAN BERG¹, JANINE WILKEN¹, STEPHAN BLOCK², and CHRISTIANE A. HELM¹ — ¹Inst. f. Physik, Uni Greifswald, 17487 Greifswald, Germany — ²Chalmers University of Technology, Gothenburg, Sweden

During times of environmental stress (e.g., UV or heat exposure), levels of reactive oxygen species (ROS) can increase dramatically. This may result in significant damage to cell structures. Here we focus on the effects of ROS on DNA.

The plasmid pBR322 (E. coli cloning vector) is attacked by free hydroxyl radicals in liquid surroundings. ROS are produced by Fenton's reaction. DNA damage is assessed by AFM Tapping Mode imaging of the plasmids in air (after adsorption onto PAH-functionalized mica). As damaged DNA strands (height 0.1 nm) are much smaller than intact DNA strands (height 0.35 nm), DNA damage can be quantified based on height distribution histograms. The amount of damaged DNA strands increases with increasing strength of radical attack, and decreases if ROS scavengers like sodium acetate are added.

CPP 19.18 Tue 9:30 P1

Direct evidence of the CT-state in organic small molecule solar cells by electroluminescence measurements — THERESA LINDERL, JULIA KRAUS, STEFAN GROB, and WOLFGANG BRÜTTING — Institut of Physics, University of Augsburg, 86135 Augsburg, Germany

The open-circuit voltage of organic solar cells is limited by the formation of a charge-transfer (CT) state at the donor-acceptor interface. Direct spectroscopic evidence of the CT-state of organic solar cells can be obtained from electroluminescence measurements.

For single layer devices the electroluminescence signal is expected to reflect the fluorescence spectra of the respective material, whereas in heterojunction devices charge carrier recombination can either occur on one of the constituents or from the CT-state. We compare spectroscopic signatures of planar and bulk heterojunction organic solar cells based on small molecules to the signal of single layer devices of the individual components.

For voltages just above the open-circuit voltage V_{oc} an additional feature in the low energy part of the spectrum can be detected, that can not be attributed to any of the used materials. We interpret this additional feature as the transition from the interfacial CT-state to the ground state and relate its energy to the open-circuit voltage of solar cells.

CPP 19.19 Tue 9:30 P1

Analysis of higher recombination orders in organic bulk heterojunction solar cells — JĘDRZEJ SZMYTKOWSKI — Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Gdańsk, Poland

Recently, it has been experimentally demonstrated that an order of nongeminate recombination exceeds two in some types of organic bulk heterojunction donor-acceptor structures. This result is different than for the case of bimolecular recombination described by Langevin theory. Although several theoretical explanations of this effect have been presented, the origin of higher recombination orders is still questionable. In this work, we analyze the process of interaction between an exciton and a polaron and its role in the increasing of recombination order. The influence of a charge concentration effect on mobility is discussed.

CPP 19.20 Tue 9:30 P1

Performance of P3HT:PCBM solar cells modified with iron oxide nanoparticles — DANIEL MOSEGUÍ GONZÁLEZ and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department - LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching

Among the different systems studied in organic solar cells, the combination of P3HT:PCBM has received the highest attention. Recently, the performance of such devices under magnetic stress has been investigated. In the case of organic electronic devices, the addition of magnetic fields can be achieved via the incorporation of iron oxide nanoparticles, which has been reported as a factor influencing the de-

vice performance [1]. Magnetic fields, amongst other effects, alter the position of the molecular energy levels, allowing "a priori" forbidden spin transitions. Moreover, the presence of heavy metals increases the L-S coupling in the system, increasing the rate of intersystem crossing. The aim of the present investigation is to characterize through which channels the presence of iron oxide nanoparticles affects the performance of P3HT:PCBM based solar cells. The morphology evolution is tracked with scattering techniques. Spectral behavior and electrical response of devices are also investigated.

[1] Zhang et al., Sol. Energ. Mat. Sol. Cells, 95 (2011) 2880-2885

CPP 19.21 Tue 9:30 P1

Investigation on enhanced efficiency introduced by solvent treatment in PTB7:PC71BM bulk heterojunction organic photovoltaics — ●SHUAI GUO¹, BIYE CAO¹, WEIJIA WANG¹, JEAN-FRANÇOIS MOULIN², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748, Garching — ²Helmholtz Zentrum Geesthacht, MLZ, Lichtenbergstr. 1, 85747 Garching

Organic photovoltaics have become of major interest in fundamental researches as well as in applications. Among all the parameters governing the device performance, the morphology of active layers in organic solar cells is of highest importance. In this work the most efficient bulk heterojunction (BHJ) system PTB7:PC71BM with and without solvent treatment is thoroughly investigated. The surface structure of each film is accessed via AFM, and the depth profile of the inner film morphology is revealed by the advanced neutron scattering technique GISANS. Consequently, the complete active layer is probed. The different morphologies formed from solvent treatment are determined and compared with the corresponding performance of each system.

CPP 19.22 Tue 9:30 P1

Synthesis of porous anatase titania nanostructures by block-copolymer assisted sol-gel method — ●LIN SONG, MARTIN A. NIEDERMEIER, VOLKER KÖRSTGENS, DANIEL MOSEGUÍ GONZÁLEZ, YUAN YAO, WEIJIA WANG, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Hybrid solar cells, consisting of conjugated polymers and n-type inorganic nanocrystals (such as titania), have received great attention due to the combination of advantages such as low cost, high electron mobility, and good chemical and physical stability. To obtain high efficiency, a large surface-to-volume ratio of the inorganic semiconductor is desirable, since the excitation dissociation occurs at the interface of the inorganic and the organic parts. We prepare titanium dioxide nanostructures from sol-gel synthesis assisted with a diblock copolymer templating approach. With GISAXS the inner film morphology is probed and compared with results from SEM and AFM. The nanocrystals size and phase are confirmed by XRD and GIWAXS.

CPP 19.23 Tue 9:30 P1

Hierarchically structured titania films for efficient light harvesting in dye-sensitized solar cells — ●BO SU, YICHUAN RUI, MARTIN A. NIEDERMEIER, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Due to high surface to volume ratio and their bicontinuous morphology, foam-like nanostructures are becoming more interesting in photovoltaics. To improve the power conversion efficiency, the light-trapping strategy is widely used in dye-sensitized solar cells (DSSCs) and organic photovoltaics (OPVs). In our study, we demonstrate hierarchically structured titania films, which are made by sol-gel chemistry and soft-molding method, with an additional superstructure in the sub-micrometer range. The master is prepared by photolithography. Then replica molds are made from the master with poly(dimethyl siloxane) (PDMS). Finally, the structured titania films are prepared by PDMS molds. A fairly high level of control over the final morphology is reached via this route. The morphology of these films is characterized with SEM and AFM. The optical properties are determined by UV/Vis spectroscopy and the photocurrent-voltage characteristics of DSSCs are measured.

CPP 19.24 Tue 9:30 P1

Effect of a third component addition on high efficiency organic solar cells — ●ROSA MARIA TORRADEMÉ, SHUAI GUO, BIYE CAO, WEIJIA WANG, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-

Franck-Str. 1, 85748 Garching, Germany

Rapid progress has been envisioned on the solution-processed organic bulk heterojunction (BHJ) solar cells in the past decade, and the efficiency has exceeded the threshold for commercial application of 10%. In this work the record-setting system PTB7:PC71BM is investigated regarding the influence of addition of a third component. The aim to introduce this new component is to improve the conductivity of the active layer using polymers with relatively higher crystallinity than that of the host polymer PTB7. Photophysical properties are probed with UVvis spectroscopy and PL measurements. The inner film morphology is revealed by GISAXS and the film crystallinity is probed with GIWAXS. Surface structures are probed with AFM. The device performance is probed by measuring IV-characteristics. Therefore, the influence of the third component on the performance of the solar cells as well as the structure of the active film is addressed.

CPP 19.25 Tue 9:30 P1

The influence of solvent atmosphere on bulk heterojunction solar cells — ●WEIJIA WANG¹, SHUAI GUO¹, Kuhu SARKAR¹, MARKUS SCHINDLER¹, DAVID MAGERL¹, MARTINE PHILIPP¹, JAN PERLICH², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — ²DESY, Notkestrasse 85, 22603 Hamburg

Organic solar cells have attracted tremendous attention in the last decades. Among different architectures of solar cell, the morphology called bulk heterojunction (BHJ) plays an important role as it yields high device efficiencies. Annealing or solvent additive processing is a way to optimize the morphology of BHJ films. However, if a solar cell encapsulation is taken into account, it is also crucial to figure out how solvent atmosphere, evaporated from residual solvent, affects the solar cells, especially for the one treated with solvent. Therefore, in this work, BHJ solar cells are stored in solvent atmosphere to accelerate the related aging. In order to gain the fundamental understanding of the solar cell degradation, the final structure of BHJ films is investigated with AFM and GISAXS. Additionally, the crystalline structure is investigated with GIWAXS and compared to the absorption in the visible regime.

CPP 19.26 Tue 9:30 P1

Novel structuring of organic thin films for improved absorption and performance in organic solar cells — ●JOHANNES SCHLIPF, CLAUDIA PALUMBINY, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Organic solar cells (OSC) have recently broken the 10% efficiency barrier hence they will soon become competitive with their inorganic counterparts. In addition, OSC still have huge advantages over (the commonly used) silicon solar cells, e.g. low production costs, possible fabrication on flexible substrates, as well as their good performance under diffuse and indirect light. The latter two are addressed in this work. Nano-imprint lithography is used to form novel, artificially structured organic thin films of high aspect ratio. Applying this structure in a solar cell provokes enhanced light scattering and induced light trapping in the photo-active layer for an overall better absorption particularly under oblique incident light. Furthermore, the conductivity of the commonly used PEDOT:PSS is improved by a combination of previously established methods: the addition of a fluorosurfactant (Zonyl FS-300)[1] and subsequent post-treatment with ethylene glycol [2, 3]. Thus PEDOT:PSS becomes applicable as a stand-alone transparent electrode. In total, this provides the possibility for high-performance, flexible and ITO-free devices based on already well-established materials in the field of organic electronics. [1] Vosguerichtian et al., Adv. Funct. Mater. 2012, 22, 421-428; [2] Kim et al., Adv. Funct. Mater. 2011, 21, 1076-1081; [3] Palumbiny et al. (submitted)

CPP 19.27 Tue 9:30 P1

Trap-assisted recombination in PCDTBT:PC₇₁BM blend films investigated by transient absorption — ●JEREMIAS WEINRICH¹, ANDREAS FRITZE¹, VLADIMIR DYAKONOV^{1,2}, and CARSTEN DEIBEL¹ — ¹Experimental Physics VI, Julius-Maximilian University of Würzburg, D-97074 Würzburg — ²Bavarian Centre for Applied Energy Research (ZAE Bayern e.V.), D-97074 Würzburg

Organic photovoltaic cells have the potential to be a key technology in the field of renewable energies. They are comparatively cheap and compatible to mass production, yet have a lower power conversion efficiency (PCE) compared to silicon solar cells. The low-bandgap

polymer PCDTBT, blended with PC₇₁BM as acceptor, is a promising electron donor in organic bulk heterojunction solar cells, with PCE's yielding above 6%.

Charge carrier recombination is the dominant loss mechanism in these devices, reducing the number of charge carriers before extraction at the electrodes. We performed transient absorption spectroscopy to probe the laser-pulse induced charge carrier concentration and its decay on a time scale of 10 ns to 1 ms at different pump intensities and temperatures. We discuss the charge carrier dynamics and activation energies as well as the origin of nongeminate losses in PCDTBT-based solar cells.

CPP 19.28 Tue 9:30 P1

Hybrid solar cells based on aqueous processed titania nanoparticles — ●CHRISTOPH MAYR¹, VOLKER KÖRSTGENS¹, HRISTO IGLEV², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching — ²TU München, Physik Department, LS Laser- und Röntgenphysik, James-Frank-Str. 1, 85748 Garching

One way towards 'green' solar cells is using aqueous-processed hybrid solar cells, because they require only a low energy amount in fabrication and furthermore a production without toxic organic solvents is possible. For the electron donor and acceptor we use a water soluble P3HT analogon and TiO₂ nanoparticles, respectively. The advantage of these particles is their size tuneability, their high absorption coefficient and the high surface area. Therefore a large interfacial area with the polymer is facilitated. The active layer is applied via solution casting. The final solar cells work with a decent efficiency, which we determined under AM 1.5 conditions. Moreover we investigate the thin films of the active layer with XRD and SEM measurements to characterize the crystalline structure and the surface structure, respectively.

CPP 19.29 Tue 9:30 P1

Bottom-up parametrization of macroscopic charge transport models — ●PASCAL KORDT¹, OLE STENZEL², BJÖRN BAUMEIER¹, VOLKER SCHMIDT², and DENIS ANDRIENKO¹ — ¹Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — ²Institute of Stochastics, Ulm University, Helmholtzstr. 18, 89069 Ulm, Germany

Computer simulations help to rationalize the link between macroscopic system properties and the underlying chemical structure of the material. This requires model development at different length scales, starting from microscopic, first-principles-based simulations, to lattice-based Gaussian disorder models (GDM), to drift-diffusion equations. Here we show how one can link the microscopic, mesoscopic off-lattice (stochastic), and finally the lattice-based GDM models and examine the parameters extracted from simulations at different length scales. The approach is tested on an amorphous mesophase of a dicyanovinyl-substituted quaterthiophene (DCV4T), which belongs to a family of efficient donors used in small-molecule organic solar cells.

CPP 19.30 Tue 9:30 P1

Characterization of quenching processes on the external quantum efficiency of phosphorescent organic light-emitting diodes — ●SEBASTIAN WEHRMEISTER¹, TOBIAS D. SCHMIDT¹, WOLFGANG BRÜTTING¹, DANIEL S. SETZ², THOMAS WEHLUS², ANDREAS F. RAUSCH², and THILO C. G. REUSCH² — ¹Institute of Physics, University of Augsburg, Germany — ²OSRAM Opto Semiconductors GmbH, Regensburg, Germany

Efficiency roll-off in organic light-emitting diodes (OLEDs) as result of high current densities represents a substantial drawback for technical applications. However, since high brightness is a major request for lighting purposes, high current densities are unavoidable. To identify and analyse the impact of quenching processes on the efficiency, time-resolved spectral measurements on a red phosphorescent OLED with Iridium(III)bis(2-methylidibenzo-[h]quinoxaline)(acetylacetonate) (Ir(MDQ)₂(acac)) as emitter have been performed. We probe the excited states lifetime after a short laser pulse on top of the steady-state region of a rectangular electrical pulse [1]. By continuously increasing the current density of the electrical pulse, the non-radiative decay becomes more likely and the excited states lifetime decreases. A comparison of the calculated external quantum efficiency (EQE) based on these data with direct EQE measurements reveals the influence and the origin of quenching processes on the efficiency roll-off of the device.

[1] N. C. Giebink, S. R. Forrest, Phys. Rev. B, 235215-1 (2008)

CPP 19.31 Tue 9:30 P1

Calculation of electronic transport properties through polymers — ●FLORIAN GÜNTHER¹, SIBYLLE GEMMING¹, and GOTTHARD SEIFERT² — ¹Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — ²Institute of Physical Chemistry and Electrochemistry, Dresden University of Technology, Dresden, Germany

Organic thin-film transistors producible by low-cost roll-to-roll manufacturing processes seem to be highly promising for flexible electronics. Therefore, high mobility semiconducting polymers with ambient stability, good solubility and film-forming properties are needed. Our study is turned to the calculation of the electronic transport properties through polymers consisting of conjugated thiophene based donor units and di-ketopyrrolo-pyrrol based acceptor units. Therefore, we use empirical hopping equations such as Marcus transfer theory in order to determine the mobility of holes and electrons. The parameters required for this are taken from first-principles calculations such as density functional theory and Hartree-Fock approaches.

CPP 19.32 Tue 9:30 P1

Detailed study of the charge carriers mobility in organic bulk heterojunction solar cells — ●KATRIN ANNESER¹, ANDREAS ZUSAN¹, VLADIMIR DYAKONOV^{1,2}, and CARSTEN DEIBEL¹ — ¹Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — ²Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg

Organic solar cells provide a good alternative to conventional, silicon based photovoltaics, since they are cheaper and easy to produce. A key issue for further optimization of the power conversion efficiency is to understand fundamental loss mechanisms such as charge carrier recombination. One important parameter influencing the nongeminate recombination is the charge carrier mobility. In this work we studied the mobility in bulk heterojunction solar cells based on P3HT:PC₆₀BM and low-bandgap:PC₇₀BM by different charge extraction techniques. We discuss impact of carrier concentration, field and temperature dependence of the mobility on the recombination losses.

CPP 19.33 Tue 9:30 P1

Non-adiabatic molecular dynamics of [2+2] addition reaction of C60 driven by the electron excitation. — ●ZOBAC VLADIMIR¹, HAPALA PROKOP¹, JOSE ORTEGA², JAMES LEWIS³, and PAVEL JELINEK¹ — ¹Institute of Physics, Academy of Sciences of the Czech Republic — ²Departamento de Fisica Teorica de la Materia Condensada and Condensed Matter Physics Center Universidad Autonoma de Madrid — ³Department of Physics, West Virginia University

Co-crystallizations and supramolecular assemblies are giving rise to an explosion of new crystal structures. Here we report theoretical study of [2+2] addition mechanism of C60 molecules induced by the electron excitation. These phenomena need to describe not only ground state potential energy surface (PES), but also the excited one. Therefore we employ an efficient non-adiabatic molecular dynamics with electronic transitions using DFT local orbital formalism, which evolves simultaneously the ions and electrons. We will discuss the mechanism of the [2+2] addition and the yield as function of distance and fullerenes orientations.

CPP 19.34 Tue 9:30 P1

Electronic excitations in push-pull oligomers and their complexes with fullerene — ●BJÖRN BAUMEIER¹, MICHAEL ROHLFING², and DENIS ANDRIENKO¹ — ¹Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz — ²Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

We present a comparative study of excited states in push-pull oligomers of PCPDTBT and PSBTBT and prototypical complexes with a C₆₀ acceptor using GW-BSE. We analyze oligomers up to a length of 5 nm and find that, for both materials, the absorption energy saturates for structures larger than two repeat units due to the localized nature of the excitation. In the bimolecular complexes with C₆₀, the Frenkel to CT transition is exothermic and we observe a strong influence of the acceptor's position and orientation on the CT energy. Their binding energy is still of the order of 2 eV resulting from the lack of an explicit molecular environment. Embedding the donor-acceptor complex into a polarizable lattice leads to an energetic stabilization of the CT exciton by about 0.5 eV, while its binding energy is reduced to about 0.3 eV. We also identify a CT state with a more delocalized hole at higher energy, which opens another potential pathway for charge sep-

ation. For both polymers, the absorption and the driving force to form intermediate CT excitations are largely similar. These results confirm that the higher power conversion efficiency observed for solar cells using PSBTBT as donor material is rather a result of molecular packing than of the electronic structure of the polymer.

CPP 19.35 Tue 9:30 P1

Structure and performance of water soluble solar cells functionalized with non-magnetic nanoparticles — ●NURI HOHN, DANIEL MOSEGUÍ GONZÁLEZ, and PETER MÜLLER BUSCHBAUM — TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Organic solar cells (OSCs) offer a great potential due to low cost, large scale production and flexible design. For preparation of OSCs the hole conducting polymer Poly[3-(potassium-6-hexanoate)thiophene-2,5-diyl] (P3P6T) is employed. For comparability reasons with the broadly studied P3HT:PCBM system, P3P6T is combined with an also water-soluble C60 fullerene derivative. With respect to environment protection, the manufacturing process of the active layer tends towards a more friendly approach compared to common OSCs based on harmful organic solvents. Additionally, inclusion of non-magnetic nanoparticles in the above mentioned system is carried out, which is found to have a strong impact on the efficiency of organic, electronic devices. We pursue to characterize the influence of these nanoparticles on the rate of intersystem crossing, as this effect eventually leads to extended exciton lifetimes. Primary investigations address the electrical, spectral and morphological characterization.

CPP 19.36 Tue 9:30 P1

Flexibility investigations on low-temperature processed nanostructured polymer/titania hybrid films — ●TOBIAS WIDMANN, WELJIA WANG, LIN SONG, and PETER MÜLLER BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

On the way to green energy, hybrid solar cells show great potential. They combine a conducting polymer with an inorganic semiconductor and therefore have advantages of both materials. The flexibility is one of the most promising properties of hybrid solar cells, which ensures the production by a roll-to-roll process and in large scale. Hence, in this work the flexibility of low temperature processed hybrid thin films is investigated. A porous film structure is synthesized by incorporating a titania precursor into a diblock copolymer which functions as the template. Thereafter it is deposited on a flexible substrate and a bending test is implemented by a custom made machine. The alteration of the bare titania structure and the hybrid film structure due to bending is investigated with optical microscopy and SEM and correlated with photophysical properties probed with UVvis and PL.

CPP 19.37 Tue 9:30 P1

Aggregation Control in Organic Photovoltaic Blends — ●JUAN FELIPE MARTÍNEZ GRISALES^{1,2}, EVA M. HERZIG¹, and PETER MÜLLER-BUSCHBAUM² — ¹TU München, MSE, Lichtenbergstr. 4, 85748 Garching — ²TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Since the discovery of conductive polymers, organic photovoltaics has turned into a very active field of research. This is owed to the potential of the inexpensive and widely available energy of the sun and the wide range of possible applications [1]. To fully exploit organic photovoltaics for efficient energy conversion processes the morphology of the active layer is a crucial parameter [2]. For example, the charge transport properties closely depend on the aggregation state, i.e. the nanomorphology of the polymers. Exploiting the properties of selective solvents we present a method to control the aggregation of a binary photovoltaic blend via the addition of a co-solvent. The system is thoroughly investigated using microscopy, spectroscopy and scattering to gain fundamental understanding on the processes involved and to relate these to solar cell performance. [1] E. M. Herzig, P. Müller-Buschbaum, *Acta Futura*, 2013, 6, 17-24 [2] M. A. Ruderer, et al., *Soft Matter*, 2011,7, 5482-5493

CPP 19.38 Tue 9:30 P1

Surface morphology of P3HT, PCBM and blends of both — ●MARTIN DEHNERT¹, MARIO ZERSON¹, ALESSANDRO SEPE², SVEN HÜTTNER², ZHUXIA RONG², ULLRICH STEINER², and ROBERT MAGERLE² — ¹Chemische Physik, Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Germany — ²Cavendish Laboratory, JJ Thomson Avenue, Cambridge, U.K

We investigate the surface morphology and the nanomechanical properties of thin films of pure regioregular poly(3-hexylthiophene) (P3HT), [6,6]-phenyl C61-butyric acid methyl ester (PCBM) and blends of both using atomic force microscopy (AFM) operated in multi-set point intermittent contact (MUSIC) 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 at 175°C show the morphology at the film surface. Both materials form a nanocrystalline texture with 10 * 30 nm large domains, but with different nanomechanical properties and different surface roughness. The P3HT surface is covered with a 3-nm-thick, compliant surface layer whereas the PCBM surface is stiff and shows less tip indentation. The small needlelike crystals of PCBM are only visible in the attractive regime of the tip-sample-interaction. Thin films of blends of P3HT:PCBM were treated with 1,8-diiodooctane, a selective solvent for PCBM. This allows us to identify the contribution of PCBM to the microstructure at the blend-air-surface.

CPP 19.39 Tue 9:30 P1

Influence of electrochemical grown thiophenes at the anode interface of bulk hetero structure organic solar cells studied by photo-CELIV. — ●ARNE HENDEL, SIDHANT BOM, and VEIT WAGNER — Jacobs University Bremen, 28759 Bremen, Germany

The charge carrier mobility and the charge carrier density in the active layer play a crucial role in organic solar cells for the device performance. The need for long lasting and stable solar cells requires an understanding of the transport and degradation processes of the cell. By the technique of charge carrier extraction by linearly increasing voltage with an additional light source (photo-CELIV) the charge transport, the lifetime and recombination dynamics in the organic BHJ is studied, which gives insight into the charge carrier creation and extraction. An additional layer of thiophenes at the interface of PDOT-PSS and P3HT-PCBM grown by electropolymerization is beneficial to the solar cell performance. The effect of such layers is studied by photo-CELIV analysis and the reason for improvements is discussed.

CPP 19.40 Tue 9:30 P1

Combination of Raman spectroscopy and GIWAXS for the investigation of the morphology of organic solar cell materials — ●SIMON SCHMITT¹, EVA HERZIG², FRANZISKA FUCHS¹, VLADIMIR DYAKONOV^{1,3}, PETER MÜLLER-BUSCHBAUM², and CARSTEN DEIBEL¹ — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²MSE & Physik-Department, LS Funktionelle Materialien, Technische Universität München, 85747 Garching — ³ZAE Bayern, 97074 Würzburg

The efficiency of organic solar cells crucially depends on their active layer morphology and donor:acceptor phase separation. Therefore a more thorough understanding of the impact of varying preparation parameters on morphology changes is important to improve solar cell performance. In this study we combine the two complementary non-destructive scattering techniques of Raman spectroscopy and GIWAXS (grazing incidence wide-angle X-ray scattering) for the investigation of the PCDTBT:PC₇₀BM blend system. GIWAXS provides information about the molecular order whereas the Raman spectra reveal the vibrational modes of the conjugated polymer and fullerene. We discuss our experimental findings for different donor:acceptor blend ratios in view of the high degree of disorder in the polymer PCDTBT and the implications for the morphology-performance relation.

CPP 19.41 Tue 9:30 P1

Exciton quenching in inverted bilayer all polymer solar cells — ●KARL-PHILIPP STRUNK, THOMAS PFADLER, MIHAEL CORIC, JONAS WEICKERT, and LUKAS SCHMIDT-MENDE — University of Konstanz

All polymer solar cells are a promising type of emerging solar cells. As the current generating layer consists only of polymers it offers a great versatility and a potential for low cost fabrication. Here we combine the n-type polymer N2200 (also called P(NDI2OD-T2)) with different hole conducting p-type polymers to bilayered solar cells.

Absorption measurements and data about the band structure give an idea about good matching polymer combinations. Three different electron donors, namely P3HT, MDMO-PPV and F8TBT, are investigated in depth as they show a favourable band structure and a complementary absorption to N2200. As P3HT is one of the most investigated p-type polymers, bulk heterojunction solar cells from N2200:P3HT are optimized by improving the fabrication parameters and compared with bilayer solar cells of N2200:P3HT, MDMO-PPV and F8TBT.

Quantitative studies of photoluminescence in bulk heterojunction

and bilayers from all polymer combinations have been performed in order to calculate the exciton quenching rate. Quenching is strongest for the internal charge transfer (CT) state in N2200 which is an indication for a high diffusion length of the internal CT state.

CPP 19.42 Tue 9:30 P1

Cryogenic Break-Junction Measurements for the Characterization of Organic Molecules — •THOMAS GRELLMANN and ROGER WÖRDENWEBER — PGI-8, Forschungszentrum Jülich, Deutschland

A cryogenic setup was developed to characterize single organic molecules via the lithographical prepared break-junction technique. Measurements are performed in a helium-flow cryostat, with temperatures ranging from 20K to room temperature. Additionally, a magnetic field up to 0.5T can be applied. The break-junction sample consists of a coated metal substrate with a lithographical prepared gold nanobridge. Repeated bending of the substrate via a piezo crystal opens and closes the gold-bridge and molecules are trapped between the tips. This allows measuring the conductance and subsequently the IV-spectra of a single molecule. Due to the temperature range from cryogenic to room temperature the conduction mechanisms of molecules can be obtained. Conductance and nonlinear IV-curves of 1,4-Benzenedithiol at different temperatures were measured, and more complex porphyrine molecules are in examination.

CPP 19.43 Tue 9:30 P1

Control and Analysis of the interface trap density in MIS structures by surface treatments and impedance spectroscopy — •HIPPOLYTE HIRWA, STEVE PITNER, and VEIT WAGNER — Jacobs University Bremen, Germany

For high performance electronic devices, reliability and stability are crucial parameters. Reliability and stability issues in field effect transistors are mainly related to their interface properties. MIS capacitors are very useful tools for investigations of interface traps. Hence, they can be used to evaluate the effect of different surface treatments on the interface traps distribution. In order to improve interface properties in field effect transistors various surface treatments are in use. Octadecyltrichlorosilan (OTS) and Hexamethyldisilazan (HMDS) treatment of SiO₂ surfaces are commonly used. Their effects in terms of interface trap density of states and the corresponding time constants are investigated. Impedance measurements have been carried on MIS capacitors fabricated using silicon oxide as insulator with 3 different surface treatments and poly(3-hexylthiophene) as the semiconductor. With a proper equivalent circuit of our MIS structure, the interface trap density was extracted from a fit of the obtained impedance in dependence of frequency and applied DC voltage. A good agreement between the experimental results and the MIS structure model can be obtained upon taking into account the dispersive transport of the bulk and the surface potential fluctuations at the interface. The results reveal that the interface states density and energy distribution can be strongly modified by the surface treatment.

CPP 19.44 Tue 9:30 P1

The influence of co-evaporated polydimethylsiloxane oil on small molecule bulk heterojunction solar cells — •FELIX HOLZMUELLER¹, LUTZ WILDE², CHRISTIAN KOERNER¹, and KARL LEO¹ — ¹Institut für Angewandte Photophysik, Technische Universität Dresden, 01069 Dresden, Germany — ²Fraunhofer Institute for Photonic Microsystems, 01069 Dresden, Germany

For efficient organic solar cells (OSC), the morphology of donor-acceptor (DA) heterojunctions is of great importance. It can be influenced by methods like post-annealing or substrate heating during the evaporation. Furthermore Kaji et al. recently proposed a new method called "co-evaporant induced crystallization" [1]. An additive is co-evaporated during the vacuum deposition of the donor and acceptor materials. At the same time, the substrate is heated to a certain temperature to ensure that the incoming additive molecules desorb from the substrate surface after their arrival. A vapor of additive molecules forms above the substrate surface and supports the crystallization of the bulk phases. In this contribution we use this method to test the influence of co-evaporated polydimethylsiloxanes on different DA-combinations like e.g. zinc-phthalocyanine (ZnPc) and C₆₀. Grazing incidence X-Ray diffraction and X-ray reflection measurements are performed on co-evaporated bulk layers showing a significant increase of crystallinity for the C₆₀ phase in ZnPc:C₆₀ blends. Additionally, the influence of the co-evaporation method on the device efficiency is investigated. [1] Kaji, T. et al. (2011). Adv. Mater., 23, 3320

CPP 19.45 Tue 9:30 P1

Toolkit for microscopic charge/energy transport simulations in disordered organic semiconductors — CARL POELKING, BJORN BAUMEIER, PASCAL KORDT, JEROEN VAN DER HOLST, ANTON MELNYK, JENS WEHNER, and •DENIS ANDRIENKO — Max Planck Institute for Polymer Research, Ackermannweg 10, Mainz 55128, Germany

We present recent developments in the toolkit for charge and energy transport simulations in amorphous organic materials (VOTCA, www.votca.org) [1]. These include (i) interfaces to the GAUSSIAN, TURBOMOLE and NWCHEM packages to compute electronic couplings, internal energies and electrostatic multipoles (ii) the QM/MM scheme combined with the polarizable Thole model for evaluating energies of charged clusters embedded in a molecular environment (iii) the kinetic Monte Carlo algorithm for finite charge densities. The methods are illustrated by studying processes at a donor-acceptor interface of dicyanovinyl-substituted quaterthiophene/C₆₀, a typical donor-acceptor pair used in small molecule organic solar cells [2].

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

[2] M. Schrader, R. Fitzner, M. Hein, C. Elschner, B. Baumeier, M. Riede, K. Leo, P. Baeuerle, D. Andrienko, J. Am. Chem. Soc., 134, 6052, 2012

CPP 19.46 Tue 9:30 P1

AFM, STXM, and TEM studies of DCV-5T:C₆₀ absorber layers for highly efficient organic solar cells — •TOBIAS MÖNCH¹, PETER WARNICKE³, PETER FORMANEK², CHRISTIAN KÖRNER¹, and KARL LEO¹ — ¹TU Dresden, IAPP, Dresden — ²Leibniz-Institut für Polymerforschung Dresden e.V., Dresden — ³Paul Scherrer Institut, Villigen, Schweiz

The optoelectronic properties of organic thin film solar cells are closely related to the microstructure of the self-organized, nanostructured network of donor and acceptor molecules. Hence, the microstructure plays a crucial role in the understanding and optimization of organic solar cells. Here we use multiple high-resolution (<40 nm) techniques to study the relationship between the microstructure and electronic properties of the device: scanning transmission X-ray microscopy (STXM), photoconductive atomic force microscopy (pcAFM), and transmission electron microscopy (TEM) were used to study local chemical composition, local charge transport, and local crystallinity, respectively. Utilizing these techniques we study the impact of in-vacuo substrate heating on the phase separation of DCV-5T:C₆₀ (2:1 by volume) blends, used in highly efficient organic solar cells.

CPP 19.47 Tue 9:30 P1

The impact of a varying C₆₀:C₇₀-acceptor mixing ratio on the opto-electronic properties of planar bilayer cells — •JOHANNES MAHR¹, MICHAEL BRENDEL¹, and JENS PFLAUM^{1,2} — ¹Experimental Physics VI, University of Würzburg, 97074 Würzburg — ²ZAE Bayern, 97074 Würzburg

Many small molecule organic photovoltaic cells (OPVCs) are based on the electron acceptor C₆₀. We discuss the effect of employing C₇₀ instead of C₆₀ in prototypical diindenoperylene (DIP) based planar bilayer cells. As a result the short circuit current density (j_{sc}) is increased by 25 %, whereas the other solar cell parameters such as the fill factor and the open circuit voltage remain almost unaffected. By comparison of complementary optical and electrical measurements, the gain in j_{sc} is predominantly attributed to an enhanced absorption of the higher order fullerene C₇₀. Both acceptor molecules under investigation, are created simultaneously in common fullerene synthesis procedures. The cost extensive step to obtain pure C₆₀ and C₇₀ is the separation process of the different sizes, rendering pristine mixtures of both materials much cheaper. Therefore the effect of a varying C₆₀:C₇₀-acceptor mixing ratio, realized by co-evaporation of the two fullerenes, on the opto-electronic properties of planar bilayer cells will be elucidated in the course of this study. The occurring changes in the devices performance will be discussed in relation with structural data obtained by AFM and X-Ray diffraction. Financial support by the DFG focus program SPP1355 is gratefully acknowledged.

CPP 19.48 Tue 9:30 P1

Hierarchy of stochastic pure state wavefunctions for open quantum systems — DANIEL SÜSS¹, WALTER T. STRUNZ¹, and •ALEXANDER EISFELD² — ¹TU Dresden — ²MPI-PKS

A method is presented to efficiently solve open quantum system prob-

lems with a non-Markovian structured environment. The approach is based on the Non-Markovian quantum state diffusion (NMQSD). We derive a hierarchy of stochastic differential equations, which can be solved numerically efficient and which converges rapidly to the exact reduced density matrix. We demonstrate the usefulness of the method by considering the spin-boson problem, electronic excitation transfer in the light-harvesting Fenna-Matthews-Olson (FMO) complex and the calculation of absorption spectra of molecular aggregates.

CPP 19.49 Tue 9:30 P1

Spatially resolved defect investigation of pinholes in metal electrodes of organic photovoltaic cells — ●DANIEL FLUHR, ROLAND RÖSCH, BURHAN MUHSIN, MARCO SEELAND, and HARALD HOPPE — Institute of Physics, Technische Universität Ilmenau, 98693 Ilmenau, Germany

To date long operation lifetime remains a major problem of organic photovoltaic (OPV) devices, even though considerable improvements were achieved over the last few years. Among the reasons for solar cell degradation are impurity induced shunts, photobleaching of the organic semiconductors via oxygen and water as well as corrosion and delamination of the metal contacts due to the same reagents. In this study we focus on so-called pinholes occurring through the metal back electrode of typical devices. These pinholes provide pathways for the ingress of water and oxygen, which locally attack the metal organic interface, resulting in contact delamination. As charge injection and extraction is suppressed at delaminated areas, the active area taking part in power conversion is reduced and hence the overall efficiency suffers. We investigated the influence of different environmental conditions on the reduction of the active area of the OPV cell. Spatially resolved measurements provide information on location and size of inactive areas induced by pinholes in the metal back contact. Periodically applied non-invasive measurements during degradation of the devices reveal the dynamics and rate of growth of these defects. By looking at different device structures we find important conclusions for increasing the lifetime of organic photovoltaic devices.

CPP 19.50 Tue 9:30 P1

Optimization of Transient Photocurrent measurements for organic solar cell characterization — ●DANIEL FLUHR¹, SHAHIDUL ALAM¹, CHETAN RAJ SINGH², and HARALD HOPPE¹ — ¹Institute of Physics, Technische Universität Ilmenau, 98693 Ilmenau, Germany — ²Department of Macromolecular Chemistry I, Universität Bayreuth, 95440 Bayreuth, Germany

We report on the extension of transient photocurrent measurements for increasing the characterization range in current and time domain. The challenge is to trace the transient photocurrent over several orders of magnitude. We compare results from using various ohmic resistors with those done via a current amplifier for tracing smaller photocurrents. Here the specific resistor capacitor discharge time is a critical value, which may yield changes in the discharging dynamics. By application of the current amplifier we are able to trace the photocurrent down by several orders of magnitude. However, slight differences in the internal resistor within the current amplifier -present at different amplifier settings- complicate the quantitative analysis of the photocurrent decay. As the presence of deep traps could not be verified, further efforts are to be invested for tracing photocurrent decays over even larger current ranges. Models describing the solar cell discharge are discussed in addition.

CPP 19.51 Tue 9:30 P1

Influencing optical properties and the morphology in thin polymer films consisting of P3HT, PFO und MEH-PPV by adding small amounts of high-boiling solvent additives — ●MARKUS REICHENBERGER — Universität Bayreuth, Lehrstuhl EP2

If admixing a few volume percent of higher boiling point additives to a solution with constant polymer concentration and solvent, impact on optical transitions, electronic properties and film morphology is resulting. It is shown how this modification of the polymer solution affects thin films of P3HT. The investigation is carried out by different spectroscopical methods and various techniques of surface analysis. Diiodooctane, dichlorobenzene and octanedithiols are used as exemplary high-boiling additives. The effect of incorporating diiodooctane on films made of PFO and MEH-PPV gives approximately equivalent results as in P3HT films: By admixing a small amount of an arbitrary high boiling point additive to the polymer solution, one can control the fraction of amorphous and aggregated phase, hence potentially the charge transport, in the spin-coated polymer film.

Many a time in the literature one observes an high energetic peak at 2.12 eV, respectively 585 nm, in the photoluminescence spectrum of thin P3HT films. Recent results are able to clarify the origin of this peak.

CPP 19.52 Tue 9:30 P1

Understanding exciton dissociation at different donor-acceptor interfacial morphologies using field dependent photocurrent measurements — ●TOBIAS HAHN¹, MARLENE SCHUBERTH², PETER STROHRIEGL², and ANNA KÖHLER¹ — ¹University of Bayreuth, Exp. Physics 2 — ²Bayreuth Institute of Macromol. Research (BIMF)

Photocurrent measurements up to high electric fields may be employed to assess whether exciton dissociation prevails at an extended donor-acceptor interface with interfacial dipoles, or whether it takes place by dopant-assisted dissociation at individual donor sites. Here we have investigated the influence of acceptor diffusion into the donor layer on the contribution between these two processes, and on the impact this has on the overall solar cell efficiency. We used a donor polymer that can be cross-linked by various degrees such as to control the thermally activated diffusion of the acceptor C60 molecule into the film. Future work will focus on replacing acceptor C60 molecule by inorganic materials including an amorphous silicon layer or, eventually, silicon nanoparticles. The aim of these studies will be to understand the mechanism underlying the dissociation process at the organic / inorganic interface in hybrid solar cells.

CPP 19.53 Tue 9:30 P1

Simulations of morphology, charge transport, and optical absorption in PCPDTBT derivatives — ●ANTON MELNYK^{1,2}, BJÖRN BAUMEIER¹, DENIS ANDRIENKO¹, FLORIAN FISCHER³, SABINE LUDWIG³, MARTIN BRINKMANN⁴, and NAVAPHUN KAYUNKID⁴ — ¹Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — ²Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128, Germany — ³Institut für Polymerchemie, Universität Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart — ⁴Institut Charles Sadron, CNRS-Universität de Strasbourg, 23 rue du Loess, 67034 Strasbourg Cedex, France

Crystalline molecular arrangements in unit cells of PCPDTBT derivatives are probed using molecular dynamic simulations. Scattering patterns are calculated and compared to TEM measurements. The morphologies are then used to evaluate electronic coupling elements, energetic disorder, and finally simulate charge transport in crystalline cells. Optical excitation spectra in solid state are calculated using a QM/MM scheme based on many-body Green's function formalism, which accounts for electrostatic embedment. A link between electronic structure, morphology, and charge transport properties is established.

CPP 19.54 Tue 9:30 P1

Molecular Dynamics of Perylene Bisimide and its Conformational States — ●MANUEL HOLLFELDER and STEPHAN GEKLE — Biofluid Simulation and Modeling, Nachwuchsgruppe Theoretische Physik, Universität Bayreuth, Germany

Perylene bisimide dimers are a promising material for organic solar cells. Recent fluorescence experiments (Spreitler et al. *Phys. Chem. Chem. Phys.* (2012)) have shown evidence of three molecular states in the fluorescence spectrum. Here we use Molecular Dynamics to simulate perylene bisimide solvated in toluene and relate these three states to their three geometric conformations: A non stacked state "open" and two stacked states, where the aromatic rings are located on top of each other, which we call "para" and "anti". The stacked states are distinguished by the orientation of the perylene molecules with respect to the connection point of the alkane chain. We further investigate the stability of the three states and their transition dynamics. We find that the transition dynamics is strongly influenced by the surrounding solvent.

CPP 19.55 Tue 9:30 P1

Temperature induced conformational changes in P3HT — ●FABIAN PANZER¹, RUTH LOHWASSER², MUKUNDAN THELAKKAT², and ANNA KÖHLER¹ — ¹Experimental Physics II, University of Bayreuth, Universitätsstraße 30, 95447 Bayreuth — ²Macromolecular Chemistry I, University of Bayreuth, Universitätsstraße30, 95447 Bayreuth

P3HT is known to exist in two distinct conformations, associated with different film morphologies. These conformations consist of coiled higher-energy phase and aggregated red phase implying a more ex-

tended, planarized and better ordered conformation. These two conformations show different behaviors in absorption and fluorescence, leading to a strong impact on device performance such as OLEDs or solar-cells. We show here that the transition from one phase to the other is a phenomenon that can also be induced by temperature and occurs at a critical temperature in the polymer P3HT. We have investigated how these conformational changes depend on various material parameters such as molecular weight and polydispersity.

CPP 19.56 Tue 9:30 P1

Polarity Effects in Organic Solar Cells: The Importance of Being Long-Range — ●CARL POELKING¹, MAX TIETZE², CHRIS ELSCHNER², KARL LEO², BJÖRN BAUMEIER¹, and DENIS ANDRIENKO¹ — ¹Max Planck Institute for Polymer Research, 55128 Mainz, Germany — ²Institute for Applied Photophysics, 01062 Dresden, Germany

We highlight the staggering importance of long-range interactions in predicting energy levels in organic semiconductors. Our simulation method addresses selectively charged, polarizable systems with broken 2D periodicity. We show that the resulting polarity effects are strong enough to easily reverse the role of donor and acceptor in organic solar cells as conditioned by gas-phase energy levels. Comparing atomistic simulations to experiments, we address implications for the empirical link between molecular energy levels and open-circuit voltage and account for why the acceptor-donor-acceptor architecture is particularly suited for solar-cell applications.

CPP 19.57 Tue 9:30 P1

Surface structure of organic solar cells based on PBDTTT-C and PC71BM — ●MARIO ZERSON¹, ANDREAS ZUSAN², BJÖRN GIESEKING², CARSTEN DEIBEL², and ROBERT MAGERLE¹ — ¹Fakultät für Naturwissenschaften, 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)-thio-no[3,4-b]thiophene))-2,6-diyl] (PBDTTT-C) and PC71BM with a weight ratio of 1:1.5. The co-solvent diiodooctane (DIO) was used with ratios between 0% and 10% to increase the solubility of PC71BM. Thin films spun cast with different amounts of DIO exhibit different power conversion efficiencies and surface morphologies. We investigate the latter 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 top surface layer of the specimens. For describing and quantifying the surface morphology we use different morphological measures. We discuss the structure formation process of the blends in terms of intermixing and demixing of the donor and acceptor material during spin casting, the size of the interfacial area between donor and acceptor components, and the formation of percolation pathways for the charge carriers.

CPP 19.58 Tue 9:30 P1

Preparation and (magneto-) optical characterisation of thin film organic transition metal complexes — ●FRANK LUNGWITZ¹, MICHAEL FRONK², CAROLA MENDE³, HEINRICH LANG³, DIETRICH R.T. ZAHN², and GEORGETA SALVAN² — ¹Physics Department, Chemnitz University of Technology, Chemnitz, Germany, now at HZDR, Dresden-Rossendorf, Germany — ²Physics Department, Chemnitz

University of Technology, Chemnitz, Germany — ³Chemistry Department, Chemnitz University of Technology, Chemnitz, Germany

Characterisation of thin films of organic materials is an important step in the development of novel electronic and spintronic devices. A class of molecules which have promising perspective for application in such devices are the porphyrins. Due to their thermal stability they are evaporable in vacuum and their optical properties can be tuned by applying different sidegroups. In this work Tetra(methoxyphenyl)Porphyrins were deposited onto silicon substrates via organic molecular beam deposition (OMBD) and characterised by variable angle spectroscopic ellipsometry (VASE) and magneto-optical Kerr effect spectroscopy (MOKE) in polar geometry. The VASE data were subsequently modelled to recursively calculate the films optical constants, thickness, roughness and the molecules tilt angle with respect to the substrate. Under knowledge of the optical constants the MOKE data were used to obtain the Voigt constant which, as a conversion factor between magneto-optical effects, was employed to determine the magnetic circular dichroism (MCD) spectra of these molecules.

CPP 19.59 Tue 9:30 P1

Theoretical Investigations of Surface Relief Gratings Based on Azobenzene-Containing Polymers — ●MARCUS BÖCKMANN and NIKOS L. DOLTSINIS — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Münster, Germany

Polymers containing the azobenzene (AB) chromophore are known to exhibit photo-fluidity when exposed to inhomogeneous light fields [1]. This phenomenon results in effective mass transport and can be utilized to, e.g., create surface relief structures of distinguished shape. Recently, it has been demonstrated that specific surface relief gratings (SRGs) imprinted on the rear panel of organic photovoltaic solar cells contribute to enhanced efficiency due to trapping of incident light [2].

We investigate the photoinduced behaviour of such an active layer based on the PDO3M azo-polymer by means of multiscale molecular dynamics simulation techniques [3] making use of a molecular mechanics switch for AB photoisomerisation that we designed recently [4].

[1] P. Karageorgiev, D. Neher, B. Schulz, B. Stiller, U. Pietsch, M. Giersig, and L. Brehmer *Nature Materials* **4**, 699 (2005). [2] S.-I. Na, S.-S. Kim, J. Jo, S.-H. Oh, J. Kim, and D.-Y. Kim *Adv. Funct. Mater.* **18**, 3956 (2008). [3] M. Böckmann, D. Marx, C. Peter, L. Delle Site, K. Kremer, and N. Doltsinis, *Phys. Chem. Chem. Phys.* **10**, 1039 (2011). [4] M. Böckmann, S. Braun, N. L. Doltsinis, and D. Marx, *J. Chem. Phys.* **139**, 084108 (2013).

CPP 19.60 Tue 9:30 P1

Charge transport and energetics in merocyanine-C60 organic solar cells — ●JENS WEHNER, CARL POELKING, and DENIS ANDRIENKO — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Solar cells with efficiencies of more than 10% have recently been reported for a number of small-molecule-based organic solar cells. Among these, cells based on merocyanine dyes (easy to mass-produce and purify colorants with high absorption coefficients) offer an opportunity to make both solution and vacuum-processed devices. Due to the donor-acceptor architecture of the molecule, these compounds have large dipole moments, which in principle should impede charge mobility and change the transport levels at the donor-acceptor interface. By combining molecular dynamics simulations and quantum chemical methods we study charge transport as well as energetics at these interfaces and show why merocyanines are efficient donors in combination with C60 as an acceptor.

CPP 20: Complex Fluids and Soft Matter (original: DY, joined by CPP, BP)

Time: Tuesday 9:30–11:30

Location: ZEU 118

CPP 20.1 Tue 9:30 ZEU 118

Microrheology of shear thinning solutions — ●JUAN RUBEN GOMEZ-SOLANO^{1,2} and CLEMENS BECHINGER^{1,2} — ¹Universitaet Stuttgart, 2. Physikalisches Institut, Pfaffenwaldring 57, 70569 Stuttgart, Germany — ²Max-Planck-Institute for Intelligent Systems, 70569 Stuttgart, Germany

Colloidal probes embedded in complex fluids have been extensively employed to investigate their rheological response to small stress. However, this approach is not evident for fluids subjected to large stresses, where a variety of non-Newtonian behaviors can occur. One example of such systems are semi-dilute micellar solutions, which consist of surfactant molecules forming worm-like micelles entangled in aqueous solution. In this work, we study the motion of a colloidal probe dragged by an optical trap through a semi-dilute micellar solution of cetylpyridinium chloride. The motion of the probe creates a shear strain, which depends linearly on its mean velocity v . We measure the effective viscous drag on the probe and the fluctuations of its position as a function of v . We find that at small v , the system can be characterized by a constant viscosity, whereas the position fluctuations are statistically the same as in thermal equilibrium. However, above a certain value, the viscosity decreases as a function of v . The fluctuations of the particle position are also affected in the shear-thinning regime, and their power spectral density increases with increasing v . We find that the transition between both regimes typically occurs when the shear rate exceeds the inverse relaxation time of the entangled micelles.

CPP 20.2 Tue 9:45 ZEU 118

Shear driven instabilities in anisotropic colloidal mixtures — ●RODRIGO LUGO-FRIAS and SABINE H. L. KLAPP — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

In recent years much attention has been paid in understanding the orientational order of anisotropic hard bodies in the presence of steady shear flow [1,2]. On the other hand, sheared systems of binary mixtures of hard disc and rodlike particles have also been examined [3].

We focus in the nonequilibrium dynamics of a binary mixture of rodlike nematic polymers under shear flow. To do so, we derive from density functional theory (DFT) a mesoscopic free energy in terms of the alignment tensor for each component. We proceed to investigate their dynamical behavior using the well known mesoscopic Doi-Hess theory, which lead to a set of nonlinear differential equations [4,5,6]. Finally, we examine the total alignment of each component and its dependencies with the physical properties of the system.

- [1] S. H. L. Klapp and S. Hess, *Phys. Rev. E* **81**, 051711 (2010).
- [2] D. Strehober, H. Engel and S. H. L. Klapp, *Phys. Rev. E* **88**, 012505 (2013).
- [3] F. Tardani, L. Gentile, G. A. Ranieri and C. La Mesa, *J. Phys. Chem. C*, **117**, 8556 (2013).
- [4] S. Hess, *Z.Naturforsch. A* **31a**, 1034 (1976).
- [5] M. Doi, *J. Polym. Sci., Polym. Phys. Ed.* **19**, 229 (1981).
- [6] S. Hess and M. Kröger, *J.Phys.: Cond. Matter*, **16**, S3835 (2004).

CPP 20.3 Tue 10:00 ZEU 118

Friction of Colloidal Crystals on Commensurate and Incommensurate Substrates — ●ALEKSANDAR MIJAILOVIĆ and MICHAEL SCHMIEDEBERG — Theoretische Physik 2, Heinrich-Heine Universität, Düsseldorf, Germany

Among the fascinating properties of quasicrystals - structures that possess long range order but no translational symmetry - is the very low friction that was observed when a periodic crystal is moved over the surface of a quasicrystal [1]. Here we want to explore whether there are geometrical reasons for the small friction.

Using Brownian Dynamics simulations, the friction properties of 3D colloidal fcc-crystals on substrates with different geometries are studied. We measure the friction as a function of the drag force applied on the crystal, from which the friction coefficient is extracted. We repeat this analysis for commensurate, incommensurate periodic, and quasicrystalline substrates and investigate the effect of incommensurability as well as aperiodicity.

The (charged) colloidal particles are interacting via the Asakura-Oosawa Model, i.e., a superposition of the screened-Coulomb potential

and an attractive term, which is due to the presence of non-adsorbing polymers (not treated explicitly). Finally, our results are compared to the 2D case (cf., e.g., [2]).

1. J. Y. Park *et al.*, *Science* **309**, 1354 (2005).
2. T. Bohlein *et al.*, *Nat. Mat.* **11**, 126 (2012).

CPP 20.4 Tue 10:15 ZEU 118

Complex dynamics of a bilamellar vesicle as a simple model for leukocytes — ●BADR KAOUÏ — Theoretical Physics I, University of Bayreuth, 95440 Bayreuth, Germany — Department of Applied Physics, Eindhoven University of Technology, P. O. Box 513, 5600 MB Eindhoven, The Netherlands

The influence of the internal structure of a biological cell (e.g., a leukocyte) on its dynamics and rheology is not yet fully understood. By using 2D numerical simulations of a bilamellar vesicle (BLV) consisting of two vesicles as a cell model, we find that increasing the size of the inner vesicle (mimicking the nucleus) triggers a tank-treading-to-tumbling transition. A new dynamical state is observed, the undulating motion: the BLV inclination with respect to the imposed flow oscillates while the outer vesicle develops rotating lobes. The BLV exhibits a non-Newtonian behavior with a time-dependent apparent viscosity during its unsteady motion. Depending on its inclination and on its inner vesicle dynamical state, the BLV behaves like a solid or a liquid [Badr Kaoui, Timm Krüger and Jens Harting, *Soft Matter* **9**, 8057 (2013)].

15 min break

CPP 20.5 Tue 10:45 ZEU 118

Random Organization and Jamming within a unifying model system — ●LARS MILZ¹ and MICHAEL SCHMIEDEBERG² — ¹Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — ²Institut für Theoretische Physik 2: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, D-40204 Düsseldorf, Germany

We show that both random organization and jamming occur within the same model packing problem despite the obvious differences between these two transitions: The random organization transition describes the change from reversible to irreversible dynamics in a non-equilibrium system and the athermal jamming transition occurs when particles can no longer avoid overlaps if quenched from infinite to zero temperature.

In our unifying model system the particles are initially randomly distributed and then displaced in each step if they overlap. For random displacements we obtain a random organization transition while jamming occurs in case of deterministic shifts. For the random organization transition, we also determine the critical exponents. For the jamming transition we observe a divergence of the relaxation time of our method.

Within our model system, random organization and jamming are opposite limits of random sphere packings. In future, we want to study intermediate packing problems or mixtures or random organization and jamming that probably correspond to other equilibrium or non-equilibrium transitions.

CPP 20.6 Tue 11:00 ZEU 118

Foam morphology, frustration and topological defects in a Negatively curved Hele-Shaw geometry — ●ADIL MUGHAL, MY-FANWY EVANS, and GERD SCHRÖDER-TURK — Institut für Theoretische Physik, Friedrich-Alexander Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

We present preliminary simulations of foams and single bubbles confined in a narrow gap between parallel surfaces. Unlike previous work, in which the bounding surfaces are flat (the so called Hele-Shaw geometry), we consider surfaces with non-vanishing Gaussian curvature.

We demonstrate that the curvature of the bounding surfaces induce a geometric frustration in the preferred order of the foam. This frustration can be relieved by the introduction of topological defects (disclinations, dislocations and complex scar arrangements). We give a detailed analysis of these defects for foams confined in curved Hele-Shaw cells and compare our results with exotic honeycombs, built by bees on surfaces of varying Gaussian curvature.

Our simulations, while encompassing surfaces of constant Gaussian

curvature (such as the sphere and the cylinder), focus on surfaces with negative Gaussian curvature and in particular triply periodic minimal surfaces (such as the Schwarz P-surface and the Schoen's Gyroid surface). We use the results from a sphere-packing algorithm to generate a Voronoi partition that forms the basis of a Surface Evolver simulation, which yields a realistic foam morphology.

CPP 20.7 Tue 11:15 ZEU 118

Molecular simulation methods to compute interfacial free energies — ●RONALD BENJAMIN and JUERGEN HORBACH — Theoretical Physics II, Heinrich-Heine Universitaet, 40225 Duesseldorf, Germany
Knowledge of interfacial free energies are crucial to understanding

physical phenomena such as wetting and nucleation. In this talk we discuss several ways to extract this quantity for wall-liquid and wall-crystal interfaces. Chiefly, we discuss a new thermodynamic integration scheme developed to determine the interfacial free energy and compare it to a non-equilibrium work method and a Gibb's-Duhem type of approach known as "Gibb's-Cahn integration".

We also extended our thermodynamic integration scheme to obtain the excess free energy of a supercooled liquid in contact with amorphous walls having the same structure as the liquid. Our results shed new light on the thermodynamic behavior of supercooled liquids and help explain their slowing down in the presence of such rough walls.

CPP 21: Organic Semiconductors: Photovoltaics (original: HL, joined by CPP, DS)

Time: Tuesday 10:00–12:30

Location: POT 081

CPP 21.1 Tue 10:00 POT 081

Analytical transmission electron microscopy on hybrid solar cells based on perovskites — ●DIANA NANOVA^{1,2,4}, ANNE KATRIN KAST^{1,3,4}, CHRISTIAN MÜLLER^{1,4}, RASMUS R. SCHRÖDER^{3,4}, ROBERT LOVRINCIC^{1,4}, and WOLFGANG KOWALSKY^{1,4} — ¹Institut für Hochfrequenztechnik, TU Braunschweig — ²Kirchhoff Insitut für Physik, Universität Heidelberg — ³Cryo-EM, CellNetworks, Bioquant, Universität Heidelberg — ⁴InnovationLab GmbH, Heidelberg

Hybrid solar cells based on metal-organic perovskite absorbers are of major interest due to their remarkable power conversion efficiencies of up to 15%. Recently, it has been shown that the morphology of the perovskite itself as well as the interplay between the absorber and the mesostructured electron acceptor strongly affects the electrical properties of the device. We present a combined study of the structure-function relationship of solution processed solar cells based on mesostructured perovskites. The morphology of the solar cells was studied by analytical transmission electron microscopy (ATEM). In ATEM electron energy loss spectroscopy (EELS) and electron spectroscopic imaging (ESI) are applied in order to obtain material contrast. To be able to classify the TiO₂ and the perovskite rich areas in the cross-section of the device a series of monochromatic images in the low-loss regime was acquired. We observed significant changes in pore size, pore filling and pore distribution of the mesostructured layer depending on the annealing conditions of the perovskite. Furthermore, we correlated our results to the I-V characteristics of the solar cells.

CPP 21.2 Tue 10:15 POT 081

Alloyed zinc sulfide - copper indium disulfide nanocrystals for application in hybrid photovoltaics — ●BJÖRN KEMPKEN, NIKOLAY RADYCHEV, CHRISTOPHER KRAUSE, JIE LI, HOLGER BORCHERT, JOANNA KOLNY-OLESIK, and JÜRGEN PARISI — Carl von Ossietzky University of Oldenburg, 26111 Oldenburg

Semiconductor nanocrystals (NCs) continue to attract immense attention because of their size-dependent optical, physical, and chemical properties which causes them to be a favourable material for hybrid solar cell applications. A promising candidate for the inorganic/organic active layer is alloys of ZnS and CuInS₂ (ZCIS NCs), which on the one hand strongly absorb in the visible range up to 800 nm, and, on the other hand, belongs to the "green" type of semiconductor NCs. In the present work, high quality ZCIS NCs were synthesized and subjected to hexanethiol ligand exchange procedures. Laboratory solar cells based on blends of treated ZCIS NCs and poly[2,6-(4,4-bis-(2-ethylhexyl)-4H-cyclopenta[2,1-b;3,4-b']dithiophene)-alt-4,7(2,1,3-benzothiadiazole)] (PCPDTBT) as active layer were prepared and investigated by current-voltage and electron spin resonance measurements. Hybrid ZCIS/PCPDTBT laboratory solar cells demonstrate well pronounced diode behavior with outstanding characteristics of the open-circuit voltage which reached up to 1.2 V.

CPP 21.3 Tue 10:30 POT 081

Improving efficiency of solar power generation by combination of a sensitized mesoscopic solar cell with a thermoelectric generator — ●HANS-FRIDTJOF PERNAU, JANA HEUER, KARINA TARANTIK, ALEXANDRE JACQUOT, JAN D. KÖNIG, MARTIN JÄGLE, and KILIAN BARTHOLOMÉ — Fraunhofer IPM, Freiburg, Germany

Standard photovoltaic(PV) solar cells use only about half of the light

spectrum provided by the sun. The infrared part is not used for production of electrical energy. Even further, the infrared light heats up the pv cell and decreases thereby its efficiency. The basic idea for a combined pv and thermoelectric solar cell has been published in 2008 [1]. The improvements in thermoelectric materials and scientific work on thermoelectrics lead to new ideas for those systems [2] which will be investigated in the EU-FP7-Projekt Globasol. Within the project, a hybrid solar cell made of a sensitized mesoscopic solar cell and a thermoelectric generator (TEG) will be developed. The light of the sun is split at about 800nm. The visible and ultra violet part is transferred to the sensitized mesoscopic solar cell, the infrared part illuminates the TEG cell. With the hybrid solar cell, the full solar spectrum is exploited. We present the first modeling results of the project and the first evaluation version of the hybrid cell.

[1] T.M. Tritt, H. Böttner and L. Chen, *Thermoelectric: Direct Solar Thermal Energy Conversion*, MRS Bulletin, vol.33 (2008) pp. 366-368; [2] D. Kraemer et al., *High-performance flat panel solar thermoelectric generator with high thermal concentration*, Nature materials vol.10 (2011) pp. 532-538.

CPP 21.4 Tue 10:45 POT 081

Spin dynamics in organic solar cells measured by pulsed electrically detected magnetic resonance — ●ALEXANDER J. KUPIJAI, KONSTANTIN M. BEHRINGER, MARTIN STUTZMANN, and MARTIN S. BRANDT — Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, 85748 Garching

Organic photovoltaics are of great interest in the development of sustainable energy sources. To investigate the recombination and transport processes in organic solar cells we use the technique of pulsed electrically detected magnetic resonance (EDMR) where we measure the change of the photocurrent caused by resonant X-band microwave pulses in the presence of an external magnetic field. As test devices, we use bulk heterojunction P3HT/PCBM (poly(3-hexylthiophene-2,5-diyl) / [6,6]-phenyl C₆₁ butyric acid methyl ester) solar cells. At temperatures of 10K we are able to observe both positively and negatively charged polarons in the pulsed EDMR spectrum and can identify them as partners in a spin-dependent pair process by experiments using two microwave frequencies. Using the time resolution and sensitivity of pulsed EDMR we are able to quantify the spin dynamics of the system and measure the lifetime of parallel spin pairs, the lifetime of antiparallel spin pairs, the spin decoherence time and the coupling strength between the spin partners. All of these microscopic parameters provide valuable information for an optimization of overall solar cell efficiencies.

CPP 21.5 Tue 11:00 POT 081

Imaging the origin of S-shaped current-voltage characteristics of organic solar cells by scanning Kelvin probe microscopy — ●CHRISTIAN MÜLLER^{1,2,3}, REBECCA SAIVE^{1,2,3}, JANUSZ SCHINKE^{1,3}, ROBERT LOVRINCIC^{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

We investigated organic bilayer solar cells consisting of poly(3-hexylthiophene)/1-(3-methoxycarbonyl)propyl-1-phenyl[6,6]C₆₁ (P3HT/PCBM). Scanning Kelvin probe microscopy (SKPM) was performed on the solar cell cross sections which were exposed with a focused ion beam. We prepared the P3HT/PCBM bilayer solar cells

by solution processing. These bilayer solar cells showed normal and anomalous, S-shaped current-voltage characteristics. Using SKPM on the device cross sections, we found that in normal bilayer solar cells the potential dropped at the ITO/PEDOT:PSS contact and over the active area, whereas in S-shaped bilayer solar cells the potential dropped exclusively at the aluminium contact. This behavior confirms the assumption that S-shaped curves are caused by hindered charge transport at electrode interfaces.

Coffee break (15 min.)

CPP 21.6 Tue 11:30 POT 081

Improving the Charge Transport Parameters of Near-Infrared Absorbers — ●SEBASTIAN RADKE^{1,2}, FRANK ORTMANN^{1,2}, REINHARD SCHOLZ^{2,3}, and GIANAURELIO CUNIBERTI^{1,2,4} — ¹Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — ²Dresden Center for Computational Materials Science, TU Dresden, Germany — ³Institut für Angewandte Photo-physik, TU Dresden, Germany — ⁴Center for Advancing Electronics Dresden, TU Dresden, Germany

For an improved performance of organic tandem solar cells, efficient organic infrared absorber materials are necessary. A promising class already used successfully in organic solar cells are 4,4'-difluoro-4-bora-3a,4a-diaza-s-indacenes (BODIPYs). Based on a comparative study of the intramolecular electronic properties as well as the intermolecular coupling in the crystal phase of three potential candidates, we find that the benzannulation of the molecular core improves both electron and hole transfer. As the frontier molecular orbitals are delocalized over the entire molecule also by attaching additional functional groups to the molecular core, the intermolecular coupling and especially the performance in amorphous phase can be optimized further. However, an immobilization of these substituents is necessary to regulate an increase in the reorganization energy for hole transfer. Based on these design rules, BODIPYs with optimized charge transfer properties can be synthesized increasing also the performance of the devices.

CPP 21.7 Tue 11:45 POT 081

Qualitative und quantitative Auswertung von komplexen bildgebenden Methoden zur Degradationsuntersuchung und Qualitätskontrolle von Polymersolarzellen — ●ROLAND RÖSCH, MARCO SEELAND, DANIEL FLUHR, BURHAN MUHSIN, PETER FISCHER, ROLF ÖTTKING und HARALD HOPPE — Institut für Physik, TU Ilmenau, Deutschland

Wir berichten über beschleunigte Alterungstests an modernen organischen und polymeren Solarzellen, ergänzt durch bildgebenden Methoden, wie z.B. bildgebende Lumineszenz, Lock-in Thermographie und lichtinduziertes Kurzschlussstrommapping. Neben einer qualitativen Interpretation der Daten, ist es durch die Kombination der verschiedenen Methoden möglich, auch eine quantitative Auswertung der Dynamiken der verschiedenen Degradationsmechanismen zu erhalten. Desweiteren vergleichen wir die experimentellen Ergebnisse mit theoretischen Modellen des Ladungsträgerflusses und -Rekombination. Daraus lassen sich intrinsische Parameter der Bauelemente, wie Elektrodenwiderstand und Diodenidealitätsfaktor bestimmen. Die wichtigste Erkenntnis aus diesen Untersuchungen ist, dass die Stabilität von modernen organischen Solarzellen vor allem durch die Elektrodendegrada-

tion und die Qualität der Versiegelung begrenzt ist. Diese Arbeit liefert einen Leitfaden für weitere Verbesserungen hin zu stabilen organischen Solarzellen.

CPP 21.8 Tue 12:00 POT 081

Visualization of Lateral Phase Separation in Polymer: Fullerene Solar Cells by Quantitative Evaluation of Luminescence Imaging Measurements — ●MARCO SEELAND, CHRISTIAN KÄSTNER, and HARALD HOPPE — Institut für Physik, TU Ilmenau, Ilmenau, Germany

Luminescence imaging has evolved to a versatile characterization method for studying the laterally resolved behavior of polymer solar cells. Especially in degradation studies the use of luminescence imaging is beneficial as it is non-invasive and offers short measurement times. By either electrical or optical excitation separate characterization of the electrical contacts and the active layer is feasible. However, the data analysis so far is mainly qualitative, i.e. interpretation of the measured luminescence image by comparison with other techniques. In this work we present a quantitative analysis of electroluminescence images of laterally inhomogeneous polymer solar cells. By decoupling the local parameters within an iteration procedure this analysis allows calculation of the local current flow through and the local voltage applied to the active layer. Furthermore quantitative images of the local series resistance and the saturation current-density are achieved. The local saturation current-density contrast was found to correlate perfectly with the strong lateral phase separation occurring in PPE-PPV:PCBM based devices. Further analysis of the lateral difference in the saturation current-densities delivers information on the thermal activation of charge carriers at the donor/acceptor-interface and in the phase separated bulk.

CPP 21.9 Tue 12:15 POT 081

The influence of fullerene loading on the photogeneration in intercalated polymer: fullerene bulk heterojunction solar cells — ●ANDREAS ZUSAN¹, KOEN VANDEWAL², BENEDIKT ALLENDORF¹, NIS HAUKE HANSEN¹, JENS PFLAUM¹, MARTIN HEENEY³, ALBERTO SALLES², VLADIMIR DYAKONOV^{1,4}, and CARSTEN DEIBEL¹ — ¹Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — ²Department of Materials Science and Engineering, Stanford University, Stanford, California 94305, USA — ³Department of Chemistry, Imperial College, London, SW7 2AZ, UK — ⁴Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg

The conjugated polymer, pBTTT, allows a systematic tuning of the blend morphology by varying the acceptor material and blend ratio, making it a well-suited structural model for studying the fundamental processes in organic BHJ solar cells. To analyze the correlation between photogeneration and intercalation, we have performed time delayed collection field (TDCF) measurements and Fourier-transform photocurrent spectroscopy (FTPS) on pBTTT:PCBM devices in various stoichiometries. An increased PCBM loading resulted in a less field dependent dissociation, which we attribute to enhanced electron delocalization along extended PCBM nanophases and energetically driven spatial separation of polarons due to the presence of pure acceptor domains. The highly efficient transfer of charge carriers from the intercalated phase into the pure phase has been studied further by extending TDCF measurements to include segregated pBTTT:bisPCBM blends.

CPP 22: Focused Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale III (original: O, joined by CPP)

Time: Tuesday 10:30–13:15

Location: TRE Ma

Topical Talk

CPP 22.1 Tue 10:30 TRE Ma
Ultrafast relaxation dynamics of Hubbard nanoclusters —
 ●MICHAEL BONITZ¹, SEBASTIAN HERMANN¹, CHRISTOPHER HINZ¹, and DENIS LACROIX² — ¹Institut für Theoretische Physik und Astrophysik, CAU Kiel, Leibnizstr. 15, 24098 Kiel — ²IPN Orsay, 15 Rue Georges Clemenceau, 91406 Orsay

With the growing availability of intense short-pulse radiation sources it becomes possible to drive interacting many-particle or few-particle systems out of equilibrium in a controlled way. The subsequent relaxation and equilibration dynamics is still poorly understood. From a theory point of view these processes are complicated due to the simultaneous dynamics of the occupation functions and of binary correlations. The problem becomes even more complicated when the system has finite size and is spatially inhomogeneous [1]. The Hubbard model is a prototype for treating correlation effects in condensed matter or molecular systems fully including finite size and inhomogeneity effects. We, therefore, concentrate on the relaxation dynamics of small 1D, 2D and 3D Hubbard clusters that contain from a few to several hundred electrons. We observe a complex multi-stage relaxation behavior that depends on the external excitation, on the coupling strength and on the geometry of the system. In this talk we present results from two complementary theoretical approaches: first, from nonequilibrium Green functions where we apply the Generalized Kadanoff Baym ansatz [1] and, second, from a stochastic mean field approach.

[1] K. Balzer, and M. Bonitz, “Nonequilibrium Green’s Functions Approach to Inhomogeneous Systems”, *Lect. Notes Phys.* **867** (2013)

CPP 22.2 Tue 11:00 TRE Ma
Exact adiabatic approximation in TDDFT — ●JEIRAN JOKAR and NICOLE HELBIG — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The use of functionals from static density functional theory in an adiabatic way in a time-dependent framework is known to cause various problems due to the resulting exchange-correlation kernel being frequency independent. In order to isolate the effects which are due to the adiabatic approximation we calculate the exact static potential for two electron systems. Before using this potential in an adiabatic way in a time propagation we need to ensure that the potential is well defined also at those parts of space where the density is small as they might become more populated at a later time. We use the exact adiabatic approximation to describe Rabi oscillations, i.e. the oscillation between the ground state and an excited state when a monochromatic laser with a frequency close to the resonance is applied.

CPP 22.3 Tue 11:15 TRE Ma
Real-time propagation of coupled Maxwell-Schrödinger and time-dependent Kohn-Sham-Maxwell systems — ●RENÉ JESTÄDT¹, HEIKO APPEL¹, and ANGEL RUBIO^{1,2} — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — ²NanoBio Spectroscopy group and ETSEF, Universidad del País Vasco, San Sebastián, Spain

Based on the Riemann-Silberstein vector of the electromagnetic field, we formulate Maxwell’s equations in a symplectic spinor representation similar to the Dirac equation. This spinor representation allows us to use standard unitary propagation techniques developed for the Schrödinger equation [1] also for Maxwell’s equations and simplifies a coupled solution of Maxwell’s and Schrödinger’s equations. To illustrate our approach, we present the real-time evolution of atomic systems embedded in optical waveguides and dielectric nanostructures. The coupling of Maxwell’s equations to the time-dependent Kohn-Sham equations is a basic ingredient for the development of a time-dependent density functional theory formulation of quantum electrodynamics [2]. As an extension of our work on coupled Maxwell-Schrödinger systems, we show first steps of an implementation of Maxwell’s equations coupled to the time-dependent Kohn-Sham equations in the first principles real-space real-time code octopus [3].

[1] A. Castro et al., *J. Chem. Phys.* **121** (2004).

[2] M. Ruggenthaler, F. Mackenroth, and D. Bauer, *Phys. Rev. A* **84**, 042107 (2011); *I. Tolkatly, Phys. Rev. Lett.* **110**, 233001 (2013).

[3] X. Andrade et al., *J. Phys. Cond. Mat.* **24** (2012).

CPP 22.4 Tue 11:30 TRE Ma
Nonlinear optics by means of the dynamical Berry phase: Application to second- and third-harmonic generation — ●CLAUDIO ATTACALITE¹ and MYRTA GRUNING² — ¹Univ. Grenoble Alpes/CNRS, Institut Neel, F-38042 Grenoble, France — ²School of Mathematics and Physics, Queen’s University Belfast, Belfast BT7 1NN, Northern Ireland, UK

We present a real-time approach to study nonlinear optical properties in Condensed Matter systems that is especially suitable for crystalline solids. The equation of motions and the coupling of the electrons with the external electric field are derived from the Berry phase formulation of the dynamical polarization. Many-body effects are introduced by adding single-particle operators to the independent-particle Hamiltonian. Specifically we include crystal local field effects, renormalization of the energy levels and excitonic effects. The approach is validated by calculating the second and third harmonic generation of bulk semiconductors. Finally we present second-harmonic generation spectrum of h-BN or MoS2 monolayers and show that correlation effects double the signal intensity at the excitonic resonances with respect to the contribution from independent electronic transitions.

References: [1] Nonlinear optics from ab-initio by means of the dynamical Berry-phase <http://arxiv.org/abs/1309.4012> [2] Second Harmonic Generation in h-BN and MoS2 monolayers: the role of electron-hole interaction <http://arxiv.org/abs/1310.7459>

15 min. break

CPP 22.5 Tue 12:00 TRE Ma
Accurate Correlation Energies from Adiabatic Time-Dependent Density Functional Theory with Renormalized Kernels — ●THOMAS OLSEN¹ and KRISTIAN S. THYGESEN² — ¹Universidad del País Vasco — ²Center for Atomic-scale Materials Design (CAMD), Technical University of Denmark

We demonstrate the accuracy of electronic correlation energies obtained from the adiabatic connection and Time-Dependent Density Functional Theory (TDDFT) using a non-empirical renormalized gradient-corrected exchange-correlation kernel. The method can be viewed as a natural step beyond the Random Phase Approximation (RPA) and captures the short-range correlation effects which are poorly described in RPA. In particular, we show that for molecules and solids the renormalized kernel gives a four and five fold improvement in binding energies respectively when compared to RPA. We also consider examples of barrier heights in chemical reactions, molecular adsorption and graphene interacting with metal surfaces, which are three examples where RPA has provided highly accurate results. In these cases, our novel kernel provides results that are of equal quality or even slightly better than RPA, with a similar computational cost. We finally note that the renormalization procedure can be applied to any known semi-local exchange-correlation functional and thus defines an entire new class of adiabatic non-local functionals for ground state calculations within TDDFT.

CPP 22.6 Tue 12:15 TRE Ma
Low scaling algorithm for the random phase approximation — ●MERZUK KALTAK, JIRI KLIMEŠ, and GEORG KRESSE — University of Vienna, Computational Material Physics

The computationally most expensive step in conventional RPA implementations is the calculation of the independent particle polarizability χ . We present an RPA algorithm that calculates χ using the Green function G in real space and imaginary time. The systematic construction of optimized time and frequency grids for G is obtained by means of solving a fitting problem. Furthermore a non-uniform discrete Fourier transform between the two grids is introduced, which converges exponentially. We show that the usage of the Green function approach in combination with the optimized grids can be used for the calculation of the RPA correlation energy for large systems.

CPP 22.7 Tue 12:30 TRE Ma
Long range correlation energy from coupled atomic response functions — ●ALBERTO AMBROSETTI and ALEXANDRE TKATCHENKO — Fritz Haber Institut der MPG, Faradayweg 4-6 14195 Berlin, Ger-

many

Electron correlation is an elusive and ubiquitous energy contribution that arises from transient collective electron fluctuations. Its reliable (accurate and efficient) modeling is central to the correct description of cohesive, structural, and response properties of molecules and solids. In this regard, the main challenge is to model the long-range correlation energy beyond (semi-)local density-functional approximations. Here we propose a very efficient method to compute the long-range correlation energy for non-metallic molecules and solids within a density functional theory framework, by using coupled atomic response functions (ARF). Extending the recent MBD method [1], we separate the coupling between ARFs into short and long range, allowing for a seamless many-body treatment of weakly and strongly polarizable systems. Thorough benchmarking on large data sets including small molecules (S22, S66x8), large supramolecular complexes (S12L), molecular crystals (X23) and bulk graphite shows consistently good agreement with high level theoretical and experimental reference binding energies (within the order of 6%). The uniform accuracy for molecules and solids represents a strong validation of our method, and further confirms the importance of modeling the truly collective nature of the long-range correlation energy. [1] A. Tkatchenko et al. PRL **108** 236402 (2012).

CPP 22.8 Tue 12:45 TRE Ma

The exact Hohenberg-Kohn functional for a lattice model — ●TANJA DIMITROV¹, HEIKO APPEL¹, and ANGEL RUBIO^{1,2} — ¹Fritz-Haber-Institut der MPG, Berlin, Germany — ²NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

Standard local exchange-correlation and semi-local functionals in ground-state density functional theory are known for their shortcomings in describing correct charge transfer, dissociation energies of molecular ions, and barriers of chemical reactions [1,2]. To understand the failures of approximate functionals and to gain insight into the behavior of the exact functional, we investigate the exact solution of the many-body Schrödinger equation for a lattice model. Using exact diagonalization, we explicitly construct the exact Hohenberg-Kohn functional and the mapping from densities to wavefunctions. Besides the normal inter-system derivative discontinuity widely discussed in

the density-functional theory community, we observe a new feature of the exact functional in the low-density limit. This "intra-system derivative discontinuity" resembles the inter-system derivative discontinuity, but is within the system (work in progress [3]). The description of many physical phenomena linked to charge-transfer processes (both in the static and dynamical regimes) require a proper account of this "intra-system derivative discontinuity".

[1] A. J. Cohen et al. Science **321**, 792 (2008).

[2] P. Mori-Sanchez et al., Phys. Rev. Lett. **100**, 146401 (2008).

[3] T. Dimitrov, H. Appel, A. Rubio to be published

CPP 22.9 Tue 13:00 TRE Ma

Incorporating static correlation effects into density functional theory — NEKTARIOS N. LATHIOTAKIS¹, ●NICOLE HELBIG², NIKITAS I. GIDOPOULOS³, and ANGEL RUBIO^{4,5} — ¹Theoretical and Physical Chemistry Institute, NHRF Athens, Greece — ²Peter-Grünberg Institut, Forschungszentrum Jülich, Germany — ³Department of Physics, Durham University, United Kingdom — ⁴Nano-Bio Spectroscopy group, Universidad del País Vasco and DIPC, San Sebastian, Spain — ⁵Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

We present a novel idea that builds on the knowledge acquired in Reduced density matrix functional theory (RDMFT) to construct a density-functional scheme which accurately incorporates static and left-right correlation effects. At the same time, the new scheme preserves the high quality of a density functional description at the equilibrium and keeps the computational costs at an acceptable level comparable to the costs when using hybrid functionals. Within this scheme the natural orbitals, i.e. the eigenfunctions of the one-body density matrix, are constrained to be solutions of a single-particle Schrödinger equation with a local effective potential. This provides a natural way to connect an energy eigenvalue spectrum to the natural orbitals. This energy spectrum is found to reproduce the ionization potentials of different atoms and molecules very well. In addition, the dissociation limit of diatomic molecules is well described without the need to break any spin symmetry, i.e. this attractive feature of RDMFT is preserved. The present scheme can be easily implemented in all first principles codes for electronic structure calculations.

CPP 23: Interfaces and Thin Films III

Time: Tuesday 15:00–16:00

Location: ZEU 114

CPP 23.1 Tue 15:00 ZEU 114

Core/Shell Microparticles by Direct Thiol-Ene Photocuring — ●CHRISTIAN KUTTNER¹, HELMUT SCHLAAD², and ANDREAS FERY¹ — ¹Physical Chemistry II, University of Bayreuth, 95447 Bayreuth, Germany — ²Max-Planck Institute of Colloids and Interfaces, Colloid Chemistry, 14424 Potsdam, Germany

Many technical applications utilize composite materials, which require specific interfacial properties between their constituents for good performance. Thus polymeric modifications are desirable for interface engineering. We developed a photocuring process based on surface-initiated thiol-ene photochemistry without the need for additional photoinitiator. By this photocuring, we prepared different core/shell composite particles consisting of polymeric shells and polyorganosiloxane cores with narrow size-distributions. [1]

Thiyl radicals at the particle surface are generated upon irradiation with UVA light. [2] The initiation process was studied by a dye degradation experiment revealing continuous formation of radicals in a timeframe of 24 hours. [1] Our approach allows for a rapid and versatile modification of surfaces and the preparation of tailored core/shell particles by both *grafting-onto* deposition of copolymers and *grafting-from* polymerization. [1-3]

[1] Kuttner, C. et al. *Langmuir* (accepted), DOI: 10.1021/la4039864.

[2] Kuttner, C. et al. *ACS Appl Mater Interfaces* **2012**, 4, 3485-3492.

[3] Kuttner, C. et al. *ACS Appl Mater Interfaces* **2013**, 5, 2469-2478.

CPP 23.2 Tue 15:15 ZEU 114

Optically triggered release from a molecular container: Photoswitching in thin films of metal-organic frameworks — ●LARS HEINKE¹, MURAT ÇAKICI², STEFAN BRÄSE², and CHRISTOF WÖLL¹ —

¹Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), Karlsruhe — ²Institute of Organic Chemistry (IOC), Karlsruhe Institute of Technology (KIT), Karlsruhe

The remote control of surface properties is one of the key challenges in interfacial science. Here, we are going to show the great potential of thin porous films of metal-organic frameworks (MOFs) containing linkers with photoswitchable azobenzene side groups. The state of the azobenzene side groups can be switched by UV light from *trans* to *cis* and vice versa by visible light. This photoswitching influences the mass transfer of the guest molecules in the pores, i.e. the pores are ideally opened and closed by light. By means of liquid-phase epitaxy, SURMOFs (surface mounted metal-organic framework) with vertical compositional gradients can be synthesized. This enables the preparation of thin porous films with a passive bottom layer, which serves as a storage container, and a photoswitchable top layer serving as a valve, which opens and closes the container. After loading the porous coating with guest molecules, its release is initiated by illumination with visible light and monitored by a quartz crystal microbalance (QCM).

CPP 23.3 Tue 15:30 ZEU 114

Role of the external field on solidification process of conjugated polymer and oligomer systems — BAKIROV ARTEM¹, SHCHERBINA MAXIM¹, GRODD LINDA², MIKAYELIAN EDUARD², FRATODDI ILARIA³, VENDITTI IOLE³, RUSSO MARIA VITTORIA³, CHVALUN SERGEI¹, and ●GRIGORIAN SOUREN² — ¹Institute of Synthetic Polymeric Materials RAS, Moscow, Russia — ²Department of Physics, University of Siegen, Germany — ³Department of Chemistry and Center for Nanotechnology for Engineering (CNIS), University of Rome Sapienza, Rome, Italy

Conjugated polymers and oligomers have received an increased attention in recent years being promising materials for organic electronics.

Recently many fabrication protocols have been developed in order to enhance structural properties which in many cases have a strong influence on final device performance. We propose a non-contact way to modify structural properties during organic film solidification under external field. First a series of in situ x-ray studies using grazing incidence geometry were realized under external electric field up to 3 keV. Here a macroscopic flow is among different experimental constraints which hinders local order. Alternatively, in situ studies were performed under external magnetic field of 1.2 T. In this case a pronounced anisotropy induced by external magnetic field was found for oligomers and polythiophene-gold nanoparticle blends.

This work was supported by BMBF (project Nr 05K10PSC).

CPP 23.4 Tue 15:45 ZEU 114

Confined semiflexible chains in a good solvent: A Monte Carlo test of scaling concepts — ●HSIAO-PING HSU^{1,2} and KURT BINDER² — ¹Max-Planck-Institut für Polymerforschung, Mainz, Germany — ²Institut für Physik, Johannes Gutenberg-Universität Mainz,

Mainz, Germany

Single semiflexible polymer chains under good solvent conditions are described by self-avoiding walks (SAWs) on the square and simple cubic lattices with an additional bending energy penalty ε_b at each 90° kink along the chains. Employing the pruned-enriched Rosenbluth method (PERM), chain lengths of polymers confined in nanoslits between two hard walls that are apart from each other at a distance D are up to 10^5 [1,2]. With our large-scale Monte Carlo simulations of confined semiflexible chains, the scaling laws predicted in Flory, Daoud-de Gennes, and Odijk regimes are checked. While under weak confinement ($D \gg l_p$) the model (for very long chains) still is compatible with the Daoud-de Gennes scaling theory, for strong confinement ($D \leq l_p$) strong deviations from the predictions based on the Kratky-Porod model are found. However, Odijk's deflection length plays no role for semiflexible chains with discrete bond angles.

[1] H.-P. Hsu and K. Binder, *Soft Matter* 9, 10512 (2013).

[2] H.-P. Hsu and K. Binder, *Macromolecules* 46, 8017 (2013).

CPP 24: Transport and Confinement II

Time: Tuesday 15:00–16:00

Location: ZEU 260

CPP 24.1 Tue 15:00 ZEU 260

Anomalous diffusion in bicontinuous microemulsions as a model system for crowded environments — ●OLIVER SCHIPPER and THOMAS HELLWEG — Bielefeld University, Germany

The understanding of the diffusive behaviour of proteins in living cells is crucial for the theoretical description of biological processes. As the interior of cells or certain cell organelles is often crowded with molecules, the diffusive behaviour of proteins does not follow the normal Fick type diffusion, where the mean square displacement grows linear in time $\langle x^2 \rangle \propto t$. The diffusion is considered to be 'anomalous': $\langle x^2 \rangle \propto t^\alpha$ (with $\alpha > 1$) [1]. To better understand the dependence of the protein diffusion on a confining environment, we studied the movement of a fluorescent particle (GFP) through a bicontinuous microemulsion via fluorescence correlation spectroscopy. The sponge like network of the microemulsion, which was characterized via small angle neutron scattering, not only slows down the translational movement of the tracer particle with decreasing domain size but also changes the characteristics of the diffusion from 'Fick like' to 'anomalous'.

[1] T. J. Feder et al., *Biophysical Journal* 1996, 70, 2767-2773.

CPP 24.2 Tue 15:15 ZEU 260

Thermal Diffusivity Measured with a Single Nanoparticle — ●ANDRÉ HEBER, MARKUS SELMKE, and FRANK CICHOS — Molecular Nano-photonics Group, Universität Leipzig, Germany

The thermal transport properties in soft matter and biological systems are of high fundamental interest. As these materials are highly heterogeneous spatially resolved measurements such as thermal diffusivity measurements are necessary to gain detailed insights. In addition far-field optical read out is desired to minimize perturbations. We use

a single metallic nanoparticle that is heated by an intensity modulated resonant laser beam. This results in a thermal wave around the particle and an accompanying refractive change. The change in the refractive index is detected by a weakly absorbed laser beam. Utilizing recent progress in single particle photothermal microscopy we are able to deduce the thermal diffusivity from the action of the thermal wave on the detection laser. With single particle photothermal microscopy it is possible to measure thermal conductivities in a great variety of materials. This scheme can easily be implemented into conventional optical microscopes.

Invited Talk

CPP 24.3 Tue 15:30 ZEU 260

Ion Conducting Polymers for Fuel Cells and Batteries: Where Polymer-chemistry meets Electrochemistry — ●KLAUS-DIETER KREUER — Max-Planck-Institut für Festkörperforschung, Stuttgart

Ion conducting polymers may simply be polymers with dissolved salts, acids or bases, but they may also be ionomers or polyelectrolytes in which the ionic groups are part of the polymer structure. In both cases, ionic interactions strongly influence the formation and mobility of ionic charge carriers, selective ionic transport, the visco-elastic behavior and even nano-scale ordering. This presentation provides experimental evidence for these effects in ion conducting polymers, which are used as membrane materials in electrochemical energy conversion and storage devices (fuel-cells and batteries), and the implications for the functioning in these devices are discussed. Based on this understanding, suggestions are being made for the modification of existing and the development of new membrane types.

K.D. Kreuer Chemistry of Materials 25th anniversary issue 2014

CPP 25: Wetting, Superamphiphobicity, Micro- and Nanofluidics II

Time: Tuesday 15:00–16:00

Location: ZEU 222

Invited Talk

CPP 25.1 Tue 15:00 ZEU 222

Superhydrophobic Arrays of Functional Janus Micropillars — ●DORIS VOLLMEYER, PERIKLIS PAPAPOPOULOS, LENA MAMMEN, CLEMENS WEISS, and HANS-JUERGEN BUTT — Max Planck Institute for Polymer Research

Wetting plays an important role in a wide variety of technological, biological, and environmental processes. Currently, a lot of research is devoted to control wetting via superhydrophilic or superhydrophobic surfaces. Combining these extreme wetting states opens exciting perspectives, including fabrication of superhydrophilic-superhydrophobic patterns to precisely control the flow and shape of liquids. High density microarrays can be fabricated using superhydrophobic Janus micropillars with a hydrophilic functional top surface. So far it was expected that the fabrication of superhydrophobic functional Janus micropillars would be conceptually impossible as the drop should immediately wet the substrate. We manifest that the fabrication of Janus micropillars is possible. Therefore, we demonstrate that the stability of the superhydrophobic state is determined by the rim of the pillars and argue that the stability of the composite state is given by a force and not by an energy balance as widely expected. The Janus pillars possess hydrophobic sidewalls and hydrophilic silica tops. The selective surface functionalization of the top surfaces with hydrophilic fluorescent molecules is illustrated with laser scanning confocal microscopy. Indeed the functionalization does not affect the stability of the air cushions.

CPP 25.2 Tue 15:30 ZEU 222

Mode Coupling of Phonons in a Dense One-Dimensional Microfluidic Crystal — ●JEAN BAPTISTE FLEURY¹, ULF D SCHILLER², SHASHI THUTUPALLI³, GERHARD GOMPPER², and RALF SEEMANN^{1,3} — ¹Saarland University, Saarbrücken, Germany — ²Forschungszentrum Jülich, Jülich, Germany — ³Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Long-living coupled transverse and longitudinal phonon modes are ex-

plored in dense and regular arrangements of flat microfluidic droplets. The collective oscillations are driven by hydrodynamic interactions between the confined droplets and can be excited in a controlled way. Experimental results are quantitatively compared to simulation results obtained by multi-particle collision dynamics. The observed transverse modes are acoustic phonons and can be described by a linearized far-field theory, whereas the longitudinal modes arise from a non-linear mode coupling due to the lateral variation of the flow field under confinement[1].

[1]Jean-Baptiste Fleury, Ulf D Schiller, Shashi Thutupalli, Gerhard Gompper and Ralf Seemann (Submitted) arXiv:1310.3655v1

CPP 25.3 Tue 15:45 ZEU 222

Semi-Flexible dense polymer brushes in flow - simulation & theory — ●FRANK RÖMER and DMITRY A. FEDOSOV — Theoretical Soft Matter and Biophysics, Institute of Complex Systems and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany

The response of dense brushes of semi-flexible polymers to flow is of great interest in both technological and biological contexts. Examples include the glycocalyx on the endothelial surface layer in blood vessels [S. Weinbaum *et al.*, *Annu. Rev. Biomed. Eng.* **9**, 121–167, 2007] and mucus-like layers in lungs or the interior of nuclear pores. We employ smoothed dissipative particle dynamics (SDPD) [P. Español, M. Revenga, *Phys. Rev. E* **67**, 026705, 2003] simulations to study semi-flexible polymer brushes for a wide range of conditions including grafting density, polymer elasticity, and shear stress due to flow. Our simulation results are in good agreement with previous studies [Y.W. Kim *et al.*, *Macromolecules* **42**, 3650–3655, 2009], which focused on brushes with low grafting densities. We also propose a theoretical model which describes the deformation of dense semi-flexible polymer brushes in shear flow for a wide parameter range. The model allows us to predict effective deformation (height), inner density profile and hydrodynamic penetration depth (solvent velocity profile). Therefore, it is suitable to predict the effect of grafted surfaces on the flow profile in a slit or tube.

CPP 26: Organic Semiconductors: Transistors and OLEDs (original: HL, joined by CPP, DS)

Time: Tuesday 14:00–15:45

Location: POT 081

CPP 26.1 Tue 14:00 POT 081

Solution-gated organic field effect transistors: small-molecule versus polymeric materials — ●HANNAH SCHAMONI¹, ROSSELLA PORRAZZO^{1,2}, JOSE A. GARRIDO¹, and MARIA ROSA ANTOGNAZZA² — ¹Walter Schottky Institut, Technische Universität München, Deutschland — ²Center for Nanoscience Technology (CNST) of IIT@Polimi, via Pascoli 70/3, 20133 Milano, Italy

Solution-gated organic field effect transistors (SGOFETs) are promising devices for biosensing applications featuring, amongst others, low production costs. For the organic semiconductor, two different kinds of materials are typically used, namely polymers like poly(2,5-bis(3-hexadecylthiophen-2-yl)thieno[3,2-b]thiophene) (pBTTT) and small molecules like α -sexithiophene (6T). In this work, we have investigated devices of both types regarding their performance, stability, and pH and ion sensitivity. A comparison of the two approaches is presented, taking also into account the differences in processing: While polymers can be spin-coated onto the substrate, small molecules are grown using organic molecular beam deposition. Finally, we will discuss the potential of SGOFETs as light sensors to stimulate nerve cells, which can pave the way towards the development of a new generation of retinal implants.

CPP 26.2 Tue 14:15 POT 081

Light-induced switching mechanism of porphyrin-coated Si nanowire field effect transistors — ●EUNHYE BAEK¹, SEBASTIAN PREGL^{1,2}, MEHRDAD SHAYGAN³, LOTTA RÖHMILDT¹, DMITRY RYNDYK^{1,2}, LARYSA BARABAN¹, and GIANAURELIO CUNIBERTI^{1,2} — ¹Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — ²Center for Advancing Electronics Dresden, TU Dresden, Germany — ³Division of IT Convergence Engi-

neering, Pohang University of Science and Technology, Pohang, Korea

We present light-induced switching mechanism of porphyrin-coated Si nanowire field effect transistors (Si NW FETs). Si NW FETs were fabricated by bottom-up methods and show ambipolar characteristics due to thermally annealed Schottky barrier on the contact between the electrode and NW channel. Si NW FETs are functionalized by porphyrin, a key dye molecule in photosynthetic process, to have photo-sensitive operation. Porphyrin-coated devices show clear current switching under light illumination that is not shown in bare devices. Switching time and switching current ratio depend on the concentration of porphyrin. Under light irradiation, electrical properties of molecular layer are changed; increased mobile charges by photo-excitation screen electrical field from the applied bias. In addition, molecules are polarized by charge separation that build vertical field towards the NWs. The electrical charge of porphyrin layer modifies the total applied field in NW, which induces current switching according to the concentration of porphyrin.

CPP 26.3 Tue 14:30 POT 081

Lithographically processed vertical organic thin-film transistors (VOTFTs) — ●ALRUN ALINE GÜNTHER¹, HANS KLEEMANN², BJÖRN LÜSSEM³, DANIEL KASEMANN¹, and KARL LEO¹ — ¹Institut für Angewandte Photophysik, TU Dresden, George-Bähr-Str. 1, 01069 Dresden Germany — ²NovaLED AG, Tatzberg 49, 01307 Dresden, Germany — ³Department of Physics, Kent State University, Kent, OH 44242, USA

Vertical organic transistors are a novel type of organic semiconductor devices, the first of such devices having been presented by Ma *et al.* in 2004[1]. The idea of this novel device concept is to overcome the limitations often faced in conventional organic thin-film transis-

tors (OTFTs), where performance parameters (e.g. cut-off frequency or transconductance) are limited by the channel length of the OTFT. The VOTFT concept developed at IAPP[2] allows for downscaling of this channel length to the order of nanometres, while using a novel photolithography approach[3] to achieve patterning of the source electrode. In the present work, the effects of semiconductor film morphology and addition of dopant molecules are investigated for pentacene VOTFTs. It is expected that knowledge of such effects will give a more detailed insight into the fundamental functional principles of the device, as these are not yet well understood.

References [1] L. Ma et al, Appl. Phys. Lett. 85, 21 (2004) [2] H. Kleemann et al, Small, Epub ahead of print (2013) [3] H. Kleemann et al, Org. Elec. 13, 3 (2012)

CPP 26.4 Tue 14:45 POT 081

Controlling morphology of a Vertical Organic Transistor for enhanced current gain and very low operation voltages — ●FELIX KASCHURA, AXEL FISCHER, BJÖRN LÜSSEM, DANIEL KASEMANN, and KARL LEO — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden

Vertical Organic Triodes represent a novel transistor technology enabling high current densities without the need for expensive structuring techniques. These devices require a permeable base for highly efficient operation. Therefore, we place a morphology modifying gold layer underneath the organic semiconductor, which enhances charge carrier transmission and thus the current gain. We have further studied a geometry optimization of the device structure allowing to tune the built-in field of the device. This results in an increased transmission as the built-in field at the collector actively gathers charge carriers, as well as a very low minimum operation voltage - both desirable characteristics for practical applications.

CPP 26.5 Tue 15:00 POT 081

Contact Resistance Adjustment in Top-Contact Organic Field Effect Transistors by Localized Doping — ●JI-LING HOU, BJÖRN LÜSSEM, DANIEL KASEMANN, and KARL LEO — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, 01069 Dresden, Germany

The contact resistance between metal and organic interface is a key challenge for Organic Field-Effect Transistors (OFETs) when short channel lengths are used to achieve low-cost and high-frequency. In this study, bottom-gate top-contact organic field effect transistors (OFETs) with different thickness of the p-dopant 2,2-(perfluoronaphthalene-2,6-diylidene) (F6-TCNNQ) under Au electrodes were fabricated by orthogonal photolithography to further investigate their impact on contact resistance. Extracted by the transmission line method (TLM), contact resistance was found to be significantly reduced from 50 kOhm*cm to 10 kOhm*cm by adding a 1nm thin dopant layer. Doping leads to an improved injection at low gate voltages, while the contact resistance is also reduced in the undoped reference device due to the applied field at higher gate voltages. Finally, we conducted temperature dependent I-V measurement to study the change of contact resistance at lower temperature. The result shows an abrupt transition in the

linear region between 220K and 240K, which gives a direct evidence and link between contact resistance and doping effect.

CPP 26.6 Tue 15:15 POT 081

IR spectroscopic investigation of charge transfer in organic semiconductors I: Doped layers — ●TOBIAS GLASER^{1,2}, SEBASTIAN BECK^{1,2}, DAVID GERBERT^{1,2}, JOHANNES ZIMMERMANN^{1,2}, and ANNEMARIE PUCCI^{1,2,3} — ¹Kirchhoff-Institut für Physik, Universität Heidelberg — ²InnovationLab GmbH, Heidelberg — ³Centre for Advanced Materials, Universität Heidelberg

Electrochemical doping of amorphous organic semiconductors is a frequently used technique in order to increase the amount of free charge carriers and thereby the conductivity of the doped layers. But for organic semiconductors, in general very low doping efficiencies in the range of only a few percent have been reported.

We performed infrared (IR) spectroscopy under ultrahigh vacuum conditions in order to investigate the process of charge transfer in various p-doped material systems. The charge transfer in doped layers can be determined with IR spectroscopy, as the new electronic structure of the charged molecules leads to a change in bond length and bond strength within the charged molecules that therefore exhibit a different vibrational spectrum compared to the neutral molecules. The appearance of broad electronic excitations in these systems shows the formation of new electronic states due to hybridization. We investigated the behavior of these electronic states after annealing as well as after degradation of the doped layers.

Financial support from the BMBF via the MESOMERIE Project (FKZ 13N10724) is gratefully acknowledged.

CPP 26.7 Tue 15:30 POT 081

IR spectroscopic investigation of charge transfer in organic semiconductors II: Interfaces — ●SEBASTIAN BECK^{1,2}, DAVID GERBERT^{1,2}, TOBIAS GLASER^{1,2}, and ANNEMARIE PUCCI^{1,2,3} — ¹Kirchhoff-Institut für Physik, Universität Heidelberg — ²InnovationLab GmbH, Heidelberg — ³Centre for Advanced Materials, Universität Heidelberg

In organic semiconductors charge transfer (CT) is crucial for all kinds of applications but its basic mechanisms are still under severe discussion. Especially a better knowledge of CT at organic/organic and inorganic/organic interfaces is essential for the design of new electronic devices with improved performance.

In this study we want to introduce a new approach to investigate CT at interfaces by means of in situ infrared (IR) spectroscopy. We investigated the system 4,4'-bis(N-carbazolyl)-1,1'-biphenyl (CBP)/MoO₃, as a prototypical example, and spectroscopically identified charged and non-charged species of CBP molecules, that were deposited onto MoO₃. Both species can be distinguished by their specific vibrational modes in the mid IR range. The inverted layer structure with MoO₃ deposited onto CBP shows a significantly different behavior that is attributed to the diffusion of MoO₃ into the organic film.

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

CPP 27: Organic Electronics and Photovoltaics (joint session with DS/HL/O) III

Polymers, Solar Cells, OFETs, OLEDs, Spectroscopy

Time: Wednesday 9:30–12:45

Location: ZEU 260

CPP 27.1 Wed 9:30 ZEU 260

Structural Degradation of Polymer Solar Cells — ●CHRISTOPH J. SCHAFFER¹, CLAUDIA M. PALUMBINY¹, MARTIN A. NIEDERMEIER¹, CHRISTIAN JENDRZEJEWSKI¹, GONZALO SANTORO², STEPHAN V. ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department - LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — ²DESY, Notkestr. 85, 22607 Hamburg

A major challenge in organic photovoltaics (OPV) is to elongate their lifetimes. Several mechanisms of organic solar cell degradation have been proposed in literature within the last years. However, insufficient research has been done on determining the role of transitions in the nanomorphology of the active layer of bulk-heterojunction (BHJ) polymer solar cells as an aspect of degradation. These transitions would strongly affect the properties of solar cells since the active layer mor-

phology plays a crucial role in the energy conversion process.

We present a direct evidence of morphological degradation on a nanometer scale in polymeric solar cells by simultaneous in-situ GISAXS and current-voltage tracking on a running P3HT:PCBM solar cell. The loss of short-circuit current with time is fully modeled by the observed morphological transitions [1].

[1] C. J. Schaffer et al., *Adv. Mater.* **2013**, DOI: 10.1002/adma.201302854

CPP 27.2 Wed 9:45 ZEU 260

Controlling nanomorphology in bulk heterojunction solar cells via addition of third component — ●EVA M. HERZIG¹, AMMARA R. AKHTAR², ANNA NAUMANN², SHUAI GUO², GREGORY TAINTER², JIANQI ZHAN², JAN PERLICH³, STEPHAN V. ROTH³, CHRISTINE M. PAPADAKIS², and PETER MÜLLER-BUSCHBAUM² — ¹TU

München, MSE, Lichtenbergstr. 4, 85748 Garching — ²TU München, Physik-Department., James-Frank-Str. 1, 85748 Garching — ³DESY, Notkestr. 85, 22603 Hamburg

Nanomorphology and efficiency of organic solar cells are closely linked. It is therefore desirable to have control over the self-assembly process responsible for the morphology formation of the active material. Employing grazing incidence small and wide angle x-ray scattering (GISAXS & GIWAXS) as well as spectroscopy and microscopy methods allows us to characterize organic thin films on the nanoscale with high statistical relevance. Using these methods we thoroughly investigate the morphological changes upon the addition of a third polymeric component showing that the self-assembly process is altered. We find that the amount of the third component controls the phase separation in the bulk heterojunction active layer. Adjusting the preparation route to support crystallization of the active material leads to an increased solar cell performance for a tuned ternary solar cell system.

CPP 27.3 Wed 10:00 ZEU 260

Layer by layer solution processing of nanostructured all-polymer solar cells — ●THOMAS PFADLER, MIHAEL CORIC, JONAS WEICKERT, KARL-PHILIPP STRUNK, and LUKAS SCHMIDT-MENDE — University of Konstanz

Organic solar cells have the potential to become an important low-cost alternative to conventional solar cells. However, before this can happen, the energy harvesting potential of organic solar cells must become more comparable with that of the pervading technology. This research is 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 cell active material on a nanometer scale. A promising application of NIL aims to control the nanostructure of a donor-acceptor interface in an organic all-polymer device. The electron accepting polymer is structured. A stiff polymer network featuring a nanostructured topography is developed by the usage of a photoactivable crosslinker molecule (sFPA). The crosslinked polymer matrix is not dissolved during spin-coating the donor polymer allowing fully solution processed device fabrication with controlled nanostructured donor-acceptor interfaces. Target of this approach is to investigate nanostructured bi-layer devices with controlled interfaces to finally enhance the overall efficiency by maximizing the interfacial area, increasing the exciton separation yield and ensuring direct pathways to the electrodes.

CPP 27.4 Wed 10:15 ZEU 260

The role of processing additives in Organic Solar Cells after the preparation process — ●STEFAN VÄTH¹, ANDREAS BAUMANN¹, ANDREAS SPERLICH¹, CARSTEN DEIBEL¹, MILUTIN IVANOVIC², HEIKO PEISERT², THOMAS CHASSÉ², and VLADIMIR DYAKONOV^{1,3} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Eberhard Karls University Tübingen, 72076 Tübingen — ³ZAE Bayern, 97074 Würzburg

Processing additives are widely used in the preparation of new high performance bulk heterojunction organic solar cells to improve the power conversion efficiency (PCE) significantly. They act as selective solvent for fullerenes and are therefore improving the morphology of the active area. Nevertheless the question whether or not these co-solvents remain in the organic solar cells after the preparation process occurs. This question could be solved by investigating blends consisting of the material system PTB7:PC₆₀BM processed with the additives diiodooctane (DIO), octanedithiol (ODT) and without additives as reference. We used the spin sensitive measurement technique light induced Electron Paramagnetic Resonance (LESR) to distinguish between positive polarons on the polymer and negative charges on the fullerene by their different g-factors. Together with Photoelectron Spectroscopy (PES) measurements we could show that the additive DIO remains partly inside the active layer of organic solar cells even after a high vacuum preparation step. We propose that they do not only lead to an improved morphology, but also to a doping effect.

CPP 27.5 Wed 10:30 ZEU 260

Radiative and non-radiative recombination in organic solar cells — ●KRISTOFER TVINGSTEDT, PHILIP PELCHMANN, VLADIMIR DYAKONOV, and CARSTEN DEIBEL — Experimental Physics VI Julius Maximilian University of Würzburg 97074 Würzburg

Although several organic solar cells has reached close to unity internal quantum efficiency at short circuit conditions, the open circuit voltage is still very far from its potential upper limit due to substantial charge

recombination of various types, which remains to be accurately determined. In this work we evaluate the limiting mechanisms in OPVs by employing complementary steady state measurements of recombination as a function of charge carrier density by thoroughly evaluating the diode ideality factor. The diode ideality is directly related to the order of recombination and we first assess it via light intensity dependent open circuit voltage characterization under the influence of a varying temperature. We focus our study on the ratio between radiative and non-radiative recombination via the interfacial charge transfer state as determined by absolute CT electroluminescence efficiency measurements, also as a function of temperature. The charge transfer state governs the radiative recombination in OPV bulk heterojunctions and is therefore crucial to evaluate in this context. Improving the radiative efficiency of OPVs will substantially increase the open circuit voltage and eventually put these promising photovoltaic converters in efficiency parity with their inorganic counterparts.

CPP 27.6 Wed 10:45 ZEU 260

Electronic Structure of Fullerene Heterodimer in Bulk-Heterojunction Blends — ●ANDREAS SPERLICH¹, OLEG G. POLUEKTOV², JENS NIKLAS², KRISTY L. MARDIS³, and VLADIMIR DYAKONOV¹ — ¹Experimental Physics VI, Julius Maximilian University of Würzburg and ZAE Bayern, 97074 Würzburg — ²Chemical Sciences and Engineering Division, ANL, Argonne, Illinois 60439, USA — ³Department of Chemistry and Physics, Chicago State University, Chicago, Illinois 60628, USA

To increase performance of organic solar cells, the optimization of the electron-accepting fullerenes has received less attention. Here, we report an electronic structure study of a novel covalently linked C₆₀-C₇₀-heterodimer in blend with the polymer PCDTBT. Upon optical excitation of polymer:heterodimer solid films, the electron is shared between both C₆₀ and C₇₀ cages. In contrast, in the solution the electron is localized on one half of the dimer. Electronic structure calculations reveal that for the heterodimer two nearly iso-energetic minima exist, essentially the cis and trans conformers. These conformers have different edge-to-edge distance between the two cages and therefore the electron is either shared between two dimer halves (cis) or localized on one half of the heterodimer (trans). By comparison with the experimental data, we conclude that the cis conformation is preferable in films, and the trans conformation in solution. These findings demonstrate how electronic coupling of the fullerene acceptor molecules is influenced by their packing in blends, which may have an impact on the charge carrier generation efficiency in solar cells.

15 min. break

CPP 27.7 Wed 11:15 ZEU 260

Cyclic potential growth mechanism for electropolymerized polythiophenes as anode buffer layers in P3HT-PCBM solar cells — ●SIDHANT BOM, MARLIS ORTEL, and VEIT WAGNER — Research Center for Functional Materials and Nanomolecular Science, Jacobs University, Bremen, Germany

A new method for electro-polymerization of polythiophenes as anode buffer layer (ABL) is presented. The ABL is used in a bulk-heterojunction solar cell with P3HT-PCBM as active material. Electro-polymerized thiophenes (ePT) are grown electrochemically with a standard three electrodes system on conductive contacts. We find a distinct impact of the time variation of the growth potential on the obtained layer properties. A new time dependent cyclic potential electro-polymerization method is systematically compared to a standard constant potential method. AFM topography reveals that a uniform homogeneous film of ePT is obtained by the time dependent cyclic potential growth method. The devices were fabricated with a 10 nm ePT between the active layer and PEDOT:PSS with aluminum as cathode. With a cyclic potential method, about 20% enhancement in short circuit current was observed in contrast to 10% enhancement with constant potential method. Improvements by the ePT layer are attributed to better band alignment of the HOMO levels and a LUMO offset of 0.2eV which gives its electron blocking characteristics. In summary, the cyclic potential method results in a better quality of ePT layers with good homogeneity and area coverage leading to further improvements in device performance.

CPP 27.8 Wed 11:30 ZEU 260

Intrinsic charge carrier mobility in PCDTBT:PC₇₁BM blend thin films investigated by simultaneous transient absorption and transient microwave conductivity measurements —

•ANDREAS FRITZE¹, JEREMIAS WEINRICH¹, VLADIMIR DYAKONOV^{1,2}, and CARSTEN DEIBEL¹ — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²ZAE Bayern, 97074 Würzburg

PCDTBT is a promising low-bandgap polymer for photovoltaic applications that has demonstrated unique recombination dynamics compared to the model P3HT system. Usually, the recombination dynamics in organics blends is expected to be proportional to the macroscopic charge carrier mobility, which is influenced by trapping and therefore potentially depends on the charge carrier concentration. For PCDTBT blends, we want to determine if the recombination dynamics are indeed governed exclusively by the low macroscopic mobility or if it is dominated by the, high local mobility. Therefore, we performed simultaneous measurements of transient absorption (TAS) and transient microwave conductivity on PCDTBT:PC₇₁BM thin films on a 10 ns to 1 ms time scale. TAS probes the charge carrier density, whereas the microwave experiment is sensitive to the intrinsic, high frequency conductivity. By investigating the charge carrier dynamics and conductivity at different laser pump intensities and temperatures, we can separate the effects of mobility relaxation from carrier concentration dependent mobility in order to understand the dominant loss mechanism in organic solar cells.

CPP 27.9 Wed 11:45 ZEU 260

On the role of the effective mass, ground state complexes and interfacial dipoles on exciton dissociation in organic donor-acceptor systems — •ANNA KÖHLER — University of Bayreuth, Bayreuth, Germany

Efficient exciton dissociation at a donor-acceptor interface is a necessary condition for obtaining high efficiency polymeric solar cells. Despite its importance, this step is still not fully understood. A central question is how and why, after photoexcitation of the donor and transfer of an electron onto the acceptor, the e-h pair can overcome their considerable mutual Coulomb potential. Possibilities that are currently discussed include the degree of delocalization of both an exciton and a charge in a conjugated polymer, ground state charge transfer complexes as well as interfacial dipoles that may exist at the donor-acceptor interface in the ground state, and the degree of energetic and structural order/disorder. In this talk I will show how we combine insight gained from ultrafast pump-probe spectroscopy, field dependent photocurrent measurements, photoemission measurements and modeling to assess which factors control the dissociation process.

CPP 27.10 Wed 12:00 ZEU 260

Non-photochemical self-quenching mechanism in conjugated polymers revealed by control of chain length and morphology — •FLORIAN STEINER, JAN VOGELSANG, and JOHN M. LUPTON — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D- 93040 Regensburg

Unraveling the complex photophysics of multichromophoric systems like conjugated polymers (CPs) is an ongoing interdisciplinary task. Some of the pressing questions in CP photophysics are: (i) what unit absorbs and emits the light in a CP? (ii) What processes take place between the absorption and emission event? And (iii) what is the interplay between excitation energy transfer between chromophores and non-radiative fluorescence decay? Answering these questions will lead to a fundamental understanding of the photophysics of CPs, which in turn can highlight important loss mechanisms regarding the efficiency in CP-based devices, such as self-quenching.

We illustrate that control of size and morphology in combination

with several single-molecule techniques leads to a universal picture of the self-quenching mechanism in CPs by addressing these questions. As a model system we chose the device-relevant prototypical CP poly(3-hexylthiophene). Morphological control, combined with well-defined sub-populations of different sizes, enabled us to correlate a diverse set of photophysical observables (brightness, emission polarization, emission spectra, photon antibunching) with each other and the size. Finally, the increasing fluorescence self-quenching with size and morphological order is rationalized with a comprehensive photophysical model.

CPP 27.11 Wed 12:15 ZEU 260

Conformations and electronic structure of Oligo-PPEs Investigated by Pulsed Electron Paramagnetic Resonance Spectroscopy — PATRICK KORF, FRIEDERIKE SCHÜTZE, CHRISTIAN HINTZE, STEFAN MECKING, and •MALTE DRESCHER — Department of Chemistry, University of Konstanz, Germany

Poly(para-phenyleneethynylene)s (PPE) are versatile polymers that are synthetically easily accessible.

Owing to their application in organic electronics and cell microscopy their microscopic and electronic properties are of high interest.

Herein we report the investigation of the electronic structure including the photo-excited triplet state of rod-like Oligo-PPEs. The lifetime, relaxation rates and populations of the triplet sublevels are quantitatively analyzed at cryogenic temperatures in a glassy toluene matrix via time-resolved EPR with synchronized UV laser flash excitation. The photo-physical properties are studied depending on the size of the delocalized π -electron system by varying the number of repeat units in the Oligo-PPEs.

In addition, their microscopic material properties are studied in particles with confined size constituted by block copolymers of PEGylated Oligo-PPEs. The molecular conformation is investigated by EPR distance measurements in solution, in bulk material as well as in particles. The data suggest that the rod-like Oligo-PPEs are present in a collapsed state in the particles.

CPP 27.12 Wed 12:30 ZEU 260

Structural and electrical characterization of Hex-5T-Hex oligothiophene thin films during film formation — •EDUARD MIKAYELIAN¹, LINDA GRODD¹, ULLRICH PIETSCH¹, ARTEM V. BAKIROV², MAXIM A. SCHERBINA², SERGEI N. CHVALUN², and SOUREN GRIGORIAN¹ — ¹University of Siegen — ²Enikolopov Institute of Synthetic Polymeric Materials of Russian Academy of Sciences

Organic semiconductors are attractive for electronics due to the low cost processing methods and their high electrical conductivity. Thiophene based polymers and oligomers are demonstrating relatively high mobility, excellent luminescence properties which used for application in solar cells, radio-frequency identification, etc. [1, 2]. We have investigated the thiophene based oligomer Hex-5T-Hex. Structural characterization has been performed by grazing incidence x-ray diffraction (GIXD) method, in particular we probed the crystallite orientations in prefabricated thin films. The 3D structure of Hex-5T-Hex oligomer evaluated from the in-plane (010), (020) and (021) reflections is consistent with 2D structure suggested from 5T based oligomer self-assembled monolayer (SAM) [3]. Additionally, we found the (100) and (100)' reflections in out-of-plane direction characterizing two different stacking along thiophene backbone axis. In order to correlate the structural properties of oligothiophene thin films with the electrical characteristics both properties were probed simultaneously during film formation. This work was supported by BMBF, project number 05K10PSC.

CPP 28: (Hydro) Gels and Elastomers

Time: Wednesday 9:30–12:30

Location: ZEU 222

Invited Talk

CPP 28.1 Wed 9:30 ZEU 222

Rheo-imaging of Polymer Networks — ●NORBERT WILLENBACHER — Karlsruhe Institute of Technology, Germany

Combining mechanical rheometry and multi-particle tracking (MPT) optical microrheology provides insight into polymer network structure.

High absolute values but weak concentration dependence of shear moduli are generic features of Intermediate filament networks, which play a crucial role in metazoan cell mechanics. MPT experiments reveal uniform mesh sizes (0.1–1 μm), but modulus values obtained from MPT are orders of magnitude lower than those from bulk rheometry. This discrepancy is attributed to a strong entropic contribution of stretched filament strands since attractive interactions at filament contact points prevent thermal equilibration. Addition of surfactant does not affect network mesh size, but allows filament strand equilibration, and the discrepancy between MPT and bulk rheometry vanishes.

Acrylate microgels, which are used as thickeners in a broad variety of commercial products, with similar chemical composition, but different molecular architecture have been investigated. Emulsion polymerization products form uniform networks (mesh size below 100nm). In contrast, the microgel system from solution polymerization is extremely inhomogeneous. Tracer particle mobility varies by orders of magnitude. Tracers diffuse freely within microgel particles, but are elastically trapped in overlap regions. A heterogeneous microstructure with a characteristic length scale of about 10 μm can be directly visualized based on spatial distribution of tracer particle mobility.

CPP 28.2 Wed 10:00 ZEU 222

Nonlinear rheology and self-healing kinetics of supramolecular polymer network — ●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

A series of supramolecular polyisobutylenes melt samples showing self-healing properties was investigated by small angle x-ray scattering and rheological experiments in order to get a microscopic understanding of special mechanical properties. All samples were end functionalized with barbituric acids groups but had different molecular weights. Analysis of the SAXS data and linear rheology showed that the samples form a reversible network of interconnected micelles in which barbituric acids clusters act as physical cross-linking points. Startup shear experiments with large shear strain and high shear rate led to shear yielding accompanied by a fast stress relaxation, indicating failure of the cross-linked network. Small amplitude oscillatory shear measurements after shear yielding were performed to measure the recovery of network. Based on the results, we propose a two-step model for the self-healing process.

CPP 28.3 Wed 10:15 ZEU 222

Electron irradiation of gelatin hydrogels to tailor the material properties — ●EMILIA I. WISOTZKI¹, MARCEL HENNES¹, CARSTEN SCHULDT², WOLFGANG KNOLLE¹, ULRICH DECKER¹, JOSEF A. KÄS², MAREIKE ZINK², and STEFAN G. MAYR^{1,2,3} — ¹Leibniz Institute of Surface Modification (IOM), Leipzig, Germany — ²Faculty of Physics and Earth Science, Leipzig University, Leipzig, Germany — ³Translational Centre for Regenerative Medicine, Leipzig University, Germany

Gelatin is a derivative of the natural and prevalent substance collagen, making it a highly interesting biomaterial for application in a wide range of areas from biomedicine to bioengineering. Reagent-free treatment methods to tune the properties of hydrogels such as gelatin are highly desirable in order to preserve existing biocompatibility and biodegradability of the material. Gelatin hydrogels have been synthesized and subsequently electron irradiated by a 10 MeV linear accelerator, in order to alter the material properties through crosslinking. Quantification of the physical crosslinking was carried out by rheological measurements and investigation of swelling behaviour to observe hydrogel strengthening and elasticity. From this data, rubber elasticity theory and the Flory-Rehner equation for isotropically swollen elastomers were used to estimate the crosslinking densities and polymer mesh size. Fourier transform infrared spectroscopy and scanning electron microscopy were used to analyze changes of the gelatin structure with respect to the irradiation dose. Systematic approaches to

precisely tune these material properties for desired applications were demonstrated with respect to irradiation dose and gelatin concentration.

CPP 28.4 Wed 10:30 ZEU 222

Mechanical properties of magneto-sensitive elastomers with the finite shape and different particle distributions — ●DMYTRO IVANEYKO^{1,2}, VLADIMIR TOSHCHÉVNIKOV¹, MARINA SAPHIANNIKOVA¹, and GERT HEINRICH^{1,2} — ¹Technische Universität Dresden — ²Leibniz-Institut für Polymerforschung Dresden e.V.

A new theoretical formalism is developed for the studies of the mechanical behaviour of magneto-sensitive elastomers (MSEs) under a uniform external magnetic field [1]. This formalism allows to combine macroscopic continuum-mechanics and microscopic approaches for complex analysis of MSEs with different shapes and with different particle distributions. It is shown that starting from a model based on an explicit discrete particle distribution one can separate the magnetic field inside the MSE into two contributions: one which depends on the shape of the sample with finite size and the other, which depends on the local spatial particle distribution. The magneto-induced deformation and the change of elastic modulus are found to be either positive or negative, their dependences on the magnetic field being determined by a non-trivial interplay between these two contributions. Mechanical properties are studied for two opposite types of coupling between the particle distribution and the magneto-induced deformation: absence of elastic coupling and presence of strong affine coupling. Predictions of a new formalism are in a qualitative agreement with existing experimental data.

[1] D. Ivaneyko, V. Toshchevnikov, M. Saphiannikova and G. Heinrich, *Soft Matter*, submitted.

CPP 28.5 Wed 10:45 ZEU 222

Poly(ethylene glycol) based microgel particles — ●KORNELIA GAWLITZA, STEFAN WELLERT, and REGINE VON KLITZING — Stranski-Laboratorium, Institut für Chemie, Technische Universität Berlin

Due to their reversible temperature induced volume phase transition (VPT), microgels made of poly-N-Isopropylacrylamide (p-NIPAM) served as model systems for basic research and have been intensively studied, e.g. their swelling behavior and internal structure.[1],[2] The polymer p-NIPAM show cytotoxicity above the VPT temperature (VPTT) when exposed to living cells longer than 3 hours.[3] This makes them inapplicable for long-time medical applications. The problem of cytotoxicity can be overcome by the synthesis of Poly(ethylene glycol) (PEG) based microgels which are both, non-cytotoxic and thermoresponsive. In this study the size, VPTT as well as the mesh size were controlled by the amount of comonomer (OEGMA), cross-linker (EGDMA) and sugar surfactant (Glucopon 220) during the synthesis.[4] The polymer particles in bulk and at surfaces were characterized by scattering and imaging techniques. The swelling behavior at surfaces in dependence from the coverage was investigated by Atomic Force Microscopy (AFM) and ellipsometry. - [1] K. Kratz, A. Lapp, W. Eimer and T. Hellweg, *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, 2002, 197, 55 [2] K. Gawlitza, S. Turner, F. Polzer, S. Wellert, M. Karg, P. Mulvaney and R. v. Klitzing, *Physical Chemistry Chemical Physics*, 2013, 15, 15623 [3] H. Vihola, A. Laukkanen, L. Valtola, H. Tenhu and J. Hirvonen, *Biomaterials*, 2005, 26, 3055 [4] J. Lutz, *Journal of Polymer Science: Part A*, 2008, 46, 3459

15 min break

CPP 28.6 Wed 11:15 ZEU 222

Reversibly crosslinked polymer networks - A self-consistent field theory study — ●THOMAS GRUHN and HEIKE EMMERICH — Material and Process Simulation MPS, Universität Bayreuth, Germany

Reversibly crosslinked hydrogels are of great technological relevance for sensors, drug delivery and other applications. The connectivity of these polymer network may depend on external parameters like the temperature or the composition of the solvent. A large variety of microstructures can be formed if the network includes block copolymers. A system of particular interest consists of AB diblock copolymers and A and B homopolymers. We have studied the structure of this sys-

tem, using an extended version of self-consistent field theory. We consider crosslink strengths weighted by the type of monomers involved. Varying the crosslink parameters the system shows a first order phase transition from a lamellar to a hexagonal microphase. We have calculated a phase diagram and compare the structure and free energy contributions as a function of the parameters [1-3].

[1] T. Gruhn, H. Emmerich, J. Mater. Res., 28, 3079, 2013.

[2] T. Gruhn, H. Emmerich, Chemosensors 1, 43, 2013.

[3] D. Li, T. Gruhn, H. Emmerich, J. Chem. Phys. (2012), 137, 024906.

CPP 28.7 Wed 11:30 ZEU 222

Collapse and swelling of bulk polymers and polymer brushes studied by solid-state NMR — UTE BÖHME and •ULRICH SCHELER — Leibniz-Institut für Polymerforschung Dresden e.V.

Dynamic NMR, relaxation NMR and measurements of residual dipolar couplings via double quantum NMR gives access to molecular mobility over a wide range of correlation times. Combined with the detection under high-resolution solid-state NMR applying CRAMPS signals of different functional groups and in particular the solvent can be separated. The separation of solvent dynamics from the polymer is key to this investigation. Slow polymer chain dynamics clearly shows in proton transverse relaxation. The chains of collapsed poly(acrylic acid) brushes are significantly more mobile than in the bulk polymer. Upon the addition of water this dynamic difference becomes stronger and an even more mobile component appears in the brush. The temperature-dependent collapse of PNIPAM has been followed by various techniques. The combination of relaxation NMR with CRAMPS shows the polymer dynamics in the collapsed state as well. There is a continuous variation of the chain dynamics over a wide temperature range around the transition temperature as shown in proton T1rho, which is very selective for motions in the kilohertz range.

CPP 28.8 Wed 11:45 ZEU 222

Molecular modeling approach to the prediction of mechanical properties of silica-reinforced rubbers — REINHARD HENTSCHEKE¹, •JONATHAN HAGER¹ und NILS W. HOJDIS² — ¹Fachbereich Mathematik und Naturwissenschaften Bergische Universität D-42097 Wuppertal, Germany — ²Material Development, Advanced Tire Materials, Continental Reifen Deutschland GmbH D-30419 Hannover, Germany

Recently we have suggested a nano-mechanical model for dissipative loss in filled elastomer networks in the context of the Payne effect. The mechanism is based on a total inter-filler particle force exhibiting an intermittent loop, due to the combination of short-range repulsion and dispersion forces with a long-range elastic attraction. The sum of these forces leads, under external strain, to a spontaneous instability of 'bonds' between the aggregates in a filler network and attendant energy dissipation due to the 'jolt-like' motion of the aggregates involved. In this work we use molecular dynamics simulations to obtain the microscopic interactions forces between surface modified silica particles. The latter are combined with the above model to estimate both the loss modulus and the low strain storage modulus in elastomers con-

taining the aforementioned filler-compatibilizer systems. The model is compared to experimental dynamic moduli of silica filled rubbers using different compatibilizers. We find good agreement between the model predictions and the experimental moduli as function of the compatibilizer concentration.

CPP 28.9 Wed 12:00 ZEU 222

Effect and Evolution of Nanostructural Complexity in Sensitive Polymer Gels — •SEBASTIAN SEIFFERT — Helmholtz-Zentrum Berlin — Freie Universität Berlin

Sensitive gels consist of polymer networks that can react to changes in their environment. This is achieved by two different ways. One way is to use polymers that exhibit sensitive interactions with the surrounding solvent, leading to selective gel swelling and deswelling. Another way is to use gels that consist of polymers crosslinked by non-covalent bonds that can be broken and re-associated. Both classes of sensitive gels are established and used in applications. However, to make this truly useful, it is necessary to understand the relations between the gel structure, dynamics, and function.

Our group studies such relations by two complementary approaches. In one approach, we use droplet-based microfluidics to fabricate microgel particles with exquisite control on their nm-scale homogeneity. This allows us to impart custom inhomogeneities to these gel particles, offering their impact to be studied, for example, in view of microgel volume phase transitions. We also use microgels as building blocks to assemble larger gel-type materials with determined inhomogeneity. In a second approach, we create and use modular toolboxes of supramolecular polymer gels, allowing for consistent variation of the type and strength of transient chain crosslinking. These networks are probed by micro- and macro-rheology to challenge and develop models for supramolecular gel self healing.

CPP 28.10 Wed 12:15 ZEU 222

The Swelling of Olympic Gels — •MICHAEL LANG¹, JAKOB FISCHER^{1,2,3}, MARCO WERNER^{1,2}, and JENS-UWE SOMMER^{1,2} — ¹Leibniz Institute of Polymer Research Dresden, Hohe Straße 6, 01069 Dresden, Germany. — ²Institute of Theoretical Physics, Technische Universität Dresden, Zellescher Weg 17, 01062 Dresden, Germany. — ³Current address: Bio Systems Analysis Group, Jena Centre for Bioinformatics (JCB) and Department for Mathematics and Computer Sciences, Friedrich Schiller University of Jena, 07743 Jena, Germany.

The swelling equilibrium of Olympic gels is studied by Monte Carlo Simulations. We observe that gels consisting of flexible cyclic molecules of a higher degree of polymerization N show a smaller equilibrium swelling degree $Q \propto N^{-0.28} \phi_0^{-0.72}$ for the same monomer volume fraction ϕ_0 at network preparation. This observation is explained by a disinterpenetration process of overlapping non-concatenated polymers upon swelling. In the limit of a sufficiently large number of concatenations per cyclic molecule we expect that the equilibrium degree of swelling becomes proportional to $\phi_0^{-1/2}$ independent of N . Our results challenge current textbook models for the equilibrium degree of swelling of entangled polymer networks.

CPP 29: Colloids and Complex Liquids I

Structure, Stabilization

Time: Wednesday 9:30–12:45

Location: ZEU 114

CPP 29.1 Wed 9:30 ZEU 114

Periodic Average Structures of Colloidal Monolayers on 1D Quasicrystalline Substrates — •LAMISS ZAIDOUNY¹, THOMAS BOHLEIN¹, JOHANNES ROTH², and CLEMENS BECHINGER^{1,3} — ¹Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — ²Institut für Theoretische und Angewandte (ITAP), Pfaffenwaldring 57, 70550 Stuttgart, Germany — ³Max-Planck-Institut für Intelligente systems, Stuttgart, Germany

We experimentally demonstrate that a colloidal monolayer with repulsive pair interaction which is subjected to a 1D quasiperiodic substrate light potential can lead to the formation of a periodic density modulation perpendicular to the orientation of the substrate. Interestingly, the periodicity does not coincide with one of the quasiperiodic length scales and is also independent of the particle number density over a

wide range. Our findings are in quantitative agreement with the concept of periodic average structures (PAS) of quasicrystals (QC) which have been introduced by Janner, Janssen and de Wolf (1). The study of this concept in our experiments can lead to understand the QC-C transformations observed in atomic systems, as for example in metallic alloys (2,3). (1) P. M. de Wolf, T. Janssen and A. Janner. Acta Crystallogr, A37, 625, 1981 (2) E. Abe, A.P. Tsai, PRL 83,4 (1999) (3) B. Grushko, D. Holland-Moritz, R. Wittman, G. Wild, Alloys Comp. 280, 215-230 (1998)

CPP 29.2 Wed 9:45 ZEU 114

Influence of electric and magnetic fields on colloidal suspensions of anisometric pigment particles — •KATHRIN MAY¹, ALEXEY EREMIN¹, SUSANNE KLEIN², and RALF STANNARIUS¹ — ¹Otto-von-Guericke Universität, FNW/IEP/ANP, 39106 Magdeburg, Ger-

many — ²HP Laboratories, Long Down Avenue, Stoke Gifford, Bristol BS34 8QZ, UK

Suspensions of anisometric nanoparticles show a wide range of interesting characteristics, like their concentration dependent phase behavior and response to electric and magnetic fields. Specifically the electro- and magneto-optical switching by aligning the colloidal particles in electric or magnetic fields makes them good candidates for the development of new devices.

The investigated colloidal particles are rod-shaped commercial pigment particles stabilized with a polymer and suspended in dodecane. They have an aspect ratio of about 5. This anisometry leads to the formation of ordered phases at concentrations above 15 wt%. In electric AC fields, the suspension can be electrically switched. In addition, the alignment of the colloidal particles in a magnetic field is investigated. For the pure suspension, very high magnetic fields in the range of 25 T are necessary. To increase the response to magnetic fields the suspensions are doped with magnetic nanoparticles. This is expected to reduce the critical magnetic field strength needed to align the pigment particles.

CPP 29.3 Wed 10:00 ZEU 114

Self-assembly of colloids driven by disclinations in a nematic host fluid — ●MARCO G. MAZZA¹, MICHAEL MELLE², SERGEJ SCHLOTTHAUER², and MARTIN SCHOEN^{2,3} — ¹MPI-DS, Göttingen, Germany — ²TU Berlin, Berlin, Germany — ³NCSU, Raleigh NC, USA

We present Monte Carlo simulations of a pair of colloidal particles immersed in a nematic host fluid. Through a calculation of the local director field we show that a pair of homogeneous colloids with locally planar anchoring surfaces attract each other if their center-of-mass distance vector forms an angle $\theta \simeq 30^\circ$ with the far-field director. We ascribe this attraction to a change in the complex three-dimensional defect structure building around the colloids and changing as the angle varies. This result settles a long-standing discrepancy between theory and experiment.

CPP 29.4 Wed 10:15 ZEU 114

Structural anisotropy of directionally dried colloids — ●LUCAS GOEHRING¹, FRANÇOIS BOULOGNE², LUDOVIC PAUCHARD², FRÉDÉRIQUE GIORGIUTTI-DAUPHINÉ², ROBERT BOTET², RALF SCHWEINS³, MICHAEL SZTUCKI⁴, JOAQUIM LI⁵, and BERNARD CABANE⁵ — ¹MPI Dynamics and Self-Organization, Göttingen, Germany — ²University Paris-Sud, Orsay, France — ³ILL, Grenoble, France — ⁴ESRF, Grenoble, France — ⁵PMMH, ESPCI, Paris, France

There are two main routes for making materials. In many cases the liquid-solid transition results from cooling, as intermolecular forces cause atoms to settle into equilibrium positions. For particulate materials such as ceramics and coatings the usual route is, instead, through the liquid-solid transition that is caused by evaporation from a dispersion of solid particles in a volatile solvent. One often sees this transition as being driven exclusively by the loss of free volume, and the solvent disappears from the description. Here we show, however, that the flow of solvent in a directionally dried colloidal dispersion breaks the orientational symmetry of the liquid and generates a structural anisotropy. This anisotropy arises when the particles have been concentrated by the flow to the point where they are caged by their neighbours into a soft, deformable network. The dispersion then acts as a yield-stress material, and accumulates strain in the direction of solidification, which freezes into the structure of the aggregated solid. To our knowledge, such bulk structural anisotropy has never been reported before, although we show experimentally that it is a robust feature of drying, and affects the optical and mechanical properties of the final solid.

CPP 29.5 Wed 10:30 ZEU 114

Shear banding in colloidal dispersions — ●PREE-CHA KIATKIRAKAJORN^{1,2} and LUCAS GOEHRING¹ — ¹Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, D-37077 Göttingen, Germany — ²Faculty of Physics, University of Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany

During the drying of colloidal dispersions, a pattern of bands frequently appears in the film behind the drying front, and oriented at an angle of 45° to the drying front line. The nature of these bands has never been explained, although they have been suggested to be shear-banding based on a visual similarity to these in metals. Through microscopy of colloidal polystyrene (98-298 nanometers), we confirm that the bands

are associated with local shear strains. We show how defects and shear localization arises during the drying of colloidal dispersions, and how a driving force for the bands arises from the compression of the dispersions during solidification. Further, we find that the spacing of the shear bands correlates with the film thickness, suggesting a mechanical release of stress, similar to cracking. When a new shear band starts, it can propagate either forwards or backwards, at a speed much greater than the drying front speed. Adding salt (between 0-30 mM NaCl) into the drying dispersions causes a reduction in spacing and the ultimate disappearance of the shear bands. All these observations are consistent with the simple explanation that the bands are a shear-localizing instability, caused by colloidal interactions during the directional solidification of colloidal dispersions and suggest how they can be controlled or eliminated.

CPP 29.6 Wed 10:45 ZEU 114

Crystallization of quasiantiferromagnetic colloids — ●GABI STEINBACH^{1,2}, SIBYLLE GEMMING^{1,2}, and ARTUR ERBE¹ — ¹Institute of Ion Beam Physics and Materials Research, Helmholtz-Center Dresden-Rossendorf, D-01314 Dresden — ²Institute of Physics, Chemnitz University of Technology, D-09107 Chemnitz

The microscopic interactions between atomic magnetic moments determine the macroscopic magnetic properties of matter. For strongly correlated magnetic systems the local spin configuration plays a key role. High relaxation times, however, make direct investigations of dynamic processes such as crystallization very difficult. Here, we present an artificial spin system of magnetic colloids, which are often discussed as potential mesoscopic model systems for condensed matter. The very low relaxation rates of interacting colloids enable the visualization of phase transitions or crystallization processes by video microscopy. The used colloids have a predefined net magnetic moment, as analogue to the atomic spin. These micromagnets show a quasiantiferromagnetic interaction. They form two-dimensional hexagonal clusters with a spin configuration similar to the 120° antiferromagnetic Neel state in the cluster center and strong deviations along the edges. The cluster size emerged as critical parameter for the occurrence of spin defects. During the cluster growth the total magnetization of the system increased in discrete steps. Further we obtained a linear increase of the inverse spin pair correlation for particles in the center. The influence of an external constant or fluctuating magnetic field is investigated as control tool for cluster growth and defect formation.

15 min. break

CPP 29.7 Wed 11:15 ZEU 114

Birefringence Analysis of the Effect of Electric Fields on the Order-Disorder Transition Temperature in Concentrated Solutions of Block-Copolymers — ●CHRISTINE KATHREIN, CHRISTIAN PESTER, HEIKO SCHOBERTH, and ALEXANDER BÖKER — Lehrstuhl für Makromolekulare Materialien und Oberflächen, DWI an der RWTH Aachen e.V., RWTH Aachen University, D-52056 Aachen, Germany

The application of electric fields is known to stabilize the disordered phase in concentrated solutions of lamellae forming block copolymers.

We address the fundamentally-important problem of the effect of dc electric fields on the order-disorder transition (ODT) temperature in microphase separated systems by performing in-situ birefringence measurements, and we compare this approach with the conventional high-throughput small angle X-ray scattering (SAXS) method. We studied concentrated solutions of block-copolymers in non-selective solvents with varied chemical- and volume composition. For both lamella and cylinder forming block-copolymers heating through the ODT temperature is accompanied by a continuous decrease in phase retardation. Birefringence has the advantage of being a non-destructive, facile method with high-throughput capacity. Moreover, the method has a very high sensitivity in detecting small thermal changes allowing a precise determination of the phase transition temperature.

The effect of various parameters such as dielectric contrast, chain length, solvent polarity and heating rate on the electric field induced shift of the ODT temperature is evaluated. Reported results provide new insights into the physics of confined chains under external fields.

CPP 29.8 Wed 11:30 ZEU 114

Nanoparticle stabilized aqueous foams: Correlation with interfacial nanoparticle adsorption — ●ADRIAN CARL, ANNE BAN-NUSCHER, and REGINE V. KLITZING — TU Berlin, Institut für Physikalische Chemie, Straße des 17. Juni 124, 10623 Berlin

Silica nanoparticles can become effective foam stabilizers when they are partially hydrophobized. Foams were prepared from dispersions of silica nanoparticles with different degrees of hydrophobic modification by a short chain amine. The samples show strong synergistic effects in terms of foamability and foam stability compared to solutions that contain the hydrophobic amine or unmodified silica particles only. The systems were characterized at various length scales from the nanometer to the centimeter scale. We determine the contact angle of the nanoparticles at the air water interface via x-ray reflectivity. With increasing hydrophobicity, the nanoparticles form a colloidal network around the air bubbles, whereby the apparent fractal dimension of the network shows a strong effect on foamability and foam structure.

CPP 29.9 Wed 11:45 ZEU 114

Magnetic Janus Particle: What Can a Toy Model Show? — ●EKATERINA NOVAK¹ and SOFIA KANTOROVICH^{1,2} — ¹Ural Federal University, Lenin av. 51, Ekaterinburg, 620000, Russia — ²University of Vienna, Sensengasse 8, 1090, Wien, Austria

The term Janus particle was introduced already 20 years ago in [Casagrande et al., Acad. Sci. II, 1988], whereas magnetic Janus particles were synthesized only recently [Zhao et al., Adv. Mater., 2009], [S. K. Smoukov et al, Soft Matter, 2009] and it has attracted considerable attention in literature because of their unique properties, especially, in the presence of an external magnetic field [Ruditskiy et al., Soft Mater, 2013]. Magnetic Janus particles are usually micron sized and have 2 "sides", in our case - half of the particle is made of a magnetic material, and the other half of silica. The analytical microstructure investigation methods and theoretical analysis of these systems is not yet fully worked out. However, due to the similarities, one can extend and use methods for capped colloids and regular magnetic fluids (see above) to handle the systems of magnetic Janus particles both at low and room temperatures. So we propose a simple toy model in which the spherical particle is divided into two hemispheres one of which contains a point dipole parallel to the division plane. We employ computer simulations and two different theoretical approaches (DFT and ground-state calculations) to understand the influence of the dipolar position and dipole-external field coupling on the cluster topology and cluster-size distributions.

CPP 29.10 Wed 12:00 ZEU 114

Structural micro and macroproperties of the magnetic anisotropic particles systems — ●ELENA PYANZINA¹, ALLA MURATOVA¹, and SOFIA KANTOROVICH^{1,2} — ¹Ural Federal University, Lenin av. 51, 620000, Ekaterinburg, Russia — ²University of Vienna, Sensengasse 8, 1090, Wien, Austria

Magnetic anisotropic particles in the last several years became an independent fast-emerging branch of dipolar soft matter research. In this contribution we focus our attention on the magnetic particles with shape anisotropy (essentially ellipsoids), which leads to the orientation-dependent steric interparticle interaction. The magnetic part of the interaction will be characterized by simple magnetic dipole-dipole interaction, with the dipole moment being always fixed in the particle's centre of mass, but with different orientation (along/perpendicular to the main axis). We present the study of microstructure and macroscopic properties (e.g., compressibility and diffusion coefficient) for the systems with different dipole orientation and particle anisotropy. We show that cluster topology, size-distribution, and average mag-

netic moment strongly depend on the system parameters. As a result macroscopic responses of the systems drastically change with particle anisotropy and the dipole orientation. This may prove to be very important in various medical and industrial applications, where a bottom up design of materials plays a crucial part.

CPP 29.11 Wed 12:15 ZEU 114

Magnetically controlled supramolecular brushes — ●PEDRO A. SÁNCHEZ¹, JOAN J. CERDÀ², TOMÁS SINTES², and SOFIA KANTOROVICH^{1,3} — ¹University of Vienna, Sensengasse 8, 1090, Wien, Austria. — ²Instituto de Física Interdisciplinar y Sistemas Complejos (UIB-CSIC), E-07122 Palma de Mallorca, Spain. — ³Ural Federal University, Lenin av. 51, Ekaterinburg, 620000, Russia.

The creation of materials with functional surfaces is currently a key topic in nanotechnology. Numerous approaches have been proposed in recent years in order to synthesize coatings that react to different applied stimuli or environment conditions. In most cases such approaches include polymers and polyelectrolytes as building blocks of brushes with a structural behavior controlled by parameters like the temperature, pH or salt concentration of the background fluid, or the presence of an external electric field. The most recent and sophisticated systems also include colloids of diverse materials embedded or grafted in the polymeric brush, either as control or functional elements. In this context, magnetic colloids represent a promising alternative for the design of advanced functional surfaces that remains mostly unexplored. Our study is intended to determine the possibilities of magnetic colloids as the basis of supramolecular brushes that may change their properties under the control of an external magnetic field. In particular, we focus on the effects of the magnetic interactions on the structural behavior of the brushes. We employ different modeling approaches that include analytical calculations and coarse-grained computer simulations to investigate the subject.

CPP 29.12 Wed 12:30 ZEU 114

Structure and phase behavior of n-alkyl-PEO polymer micelles — ●MATTHIAS AMANN, LUTZ WILLNER, JÖRG STELLBRINK, AUREL RADULESCU, and DIETER RICHTER — JCNS-1 & ICS-1, Forschungszentrum Jülich GmbH, D-52425 Jülich

We examine the structure of star-like n-alkyl-PEO polymer micelles in water as a function of polymer concentration with small-angle neutron scattering (SANS) methods. We present a temperature-quench-experiment to determine the aggregation number N_{agg} of the micelles in the semidilute regime, exploiting the well-known unimer exchange kinetics of our model system [1]. Furthermore, we investigate the phase behavior of the model system using high resolution SANS and discuss it with regard to a theoretical phase diagram for star-polymers, based on an ultrasoft interaction potential.

We found that the aggregation number $N_{agg} = 100$ of n-alkyl-PEO micelles is independent of polymer concentration, which contradicts theoretical considerations for star-like micelles predicting a strong increase of N_{agg} above the overlap concentration ϕ^* . Near the overlap concentration ϕ^* , a phase transition from liquid to a crystalline phase was observed. By analyzing the experimental structure factor of the polymer solutions, the crystalline phase could be identified as a fcc-crystal, which is in good agreement with theory.

References: [1] Zinn et al., Soft Matter **2012**, 8, 623-626.

CPP 30: Molecular Switches and Motors at Surfaces (original: SYMS, joined by CPP, O)

Time: Wednesday 9:30–12:15

Location: HSZ 02

Invited Talk CPP 30.1 Wed 9:30 HSZ 02
Imaging and manipulation of single functional molecules on surfaces — ●LEONHARD GRILL — University of Graz, Department of Physical Chemistry, Graz, Austria

Functional molecules on surfaces and their assembly into pre-defined architectures are key challenges in nanotechnology and of interest in various fields from molecular electronics over novel materials to molecular machines. Various examples of functional molecules, studied by scanning tunneling microscopy under ultrahigh vacuum conditions will be discussed. Specifically designed molecular building blocks are connected to two-dimensional networks or one-dimensional chains [1,2], which can act as molecular wires [3,4]. On the other hand, chemical processes within individual molecular can be controlled via their environment. This was observed for molecular switches, where the atomic-scale surroundings cause drastic changes in their switching probability [5]. Recently, we could show that the rate of an intramolecular hydrogen transfer reaction can be tuned up and down by single atoms in the vicinity of the molecule [6]. Finally, a combination of the two approaches will be discussed, potentially leading to heterogeneous molecular nanostructures that contain functional molecules.

[1] L. Grill et al., *Nature Nanotech.* 2, 687 (2007); [2] L. Lafferentz et al., *Nature Chem.* 4, 215 (2012); [3] L. Lafferentz et al., *Science* 323, 1193 (2009); [4] M. Koch et al., *Nature Nanotech.* 7, 712 (2012); [5] C. Dri et al., *Nature Nanotech.* 3, 649 (2008); [6] T. Kumagai et al., *Nature Chem.*, doi: 10.1038/nchem.1804.

Invited Talk CPP 30.2 Wed 10:00 HSZ 02
Adiabatic quantum motors — ●FELIX VON OPPEN — Dahlem Center for Complex Quantum Systems, Freie Universität Berlin

Microscopically, motion is frequently dominated by fluctuations, making it a challenge to generate directed motion at the nanoscale. This challenge has motivated recent experiments striving to realize nanomotors which convert electrical signals into unidirectional translational, vibrational, or rotational motion. Frequently, these experiments rely on ac actuation or current pulses to effect the directed motion of, say, a molecule or a carbon nanotube. In this talk, I will describe an alternative dc scheme to operate a nanomotor. Our proposed adiabatic quantum motor is effectively based on operating a quantum pump in reverse, a scheme whose macroscopic counterpart has been known since antiquity and is employed in current technology. Its quantum version has remained essentially unstudied despite enormous activity on adiabatic quantum pumps. Specifically, we consider a transport current which drives the periodic motion of an adiabatic degree of freedom. We relate the work performed per cycle on the motor degree of freedom to characteristics of the complementary quantum pump and discuss the motors' efficiency. We show that in principle, there exist motors which operate solely due to quantum interference, as well as ideal quantum motors with unit efficiency. The intrinsic damping of quantum motors has a lower bound which just involves Planck's constant. While most of our considerations are based on Gedankenmotors, we will also discuss possible realizations.

Invited Talk CPP 30.3 Wed 10:30 HSZ 02
Operation of molecular devices and machines on surfaces — ●SAW WAI HLA — Center for Nanoscale Materials, Argonne National Lab, and Ohio University, USA.

A recent emergent research direction is the development of complex molecular machines suitable to operate on solid surfaces. Unlike biological counterparts, the synthetic molecular machines may tolerate a more diverse range of conditions, and thus be advantageous for the complex functions with low power consumption suitable to operate in solid state devices. Development of such molecular devices requires

testing their operation mechanisms. We use low temperature scanning tunneling microscopy, spectroscopy, and molecular manipulation schemes to investigate fundamental operations of synthetic molecular switches and molecular motors on metallic surfaces. Using inelastic electron tunneling process, individual molecules can be switched from one state to another in a controlled manner [1-4]. Controlled directional rotation of molecular motors can also be performed using the same technique. Finally, this presentation will include our latest results of controlled synchronized rotation of molecular motors on surfaces.

[1] V. Iancu, A. Deshpande, S.-W. Hla, *Nano Lett.* 6, 820-823 (2006). [2] V. Iancu, and S.-W. Hla, *Proc. Nat. Acad. Sci.* 103, 13718-13721 (2006). [3] Y.-S. Fu et al. *Nano Lett.* 12, 3931-3935 (2012). [4] U.G.E. Perera et al. *Nature Nanotechnology* 5, 46-51 (2013).

15 min. break

Invited Talk CPP 30.4 Wed 11:15 HSZ 02
Driving and Controlling Molecular Surface Rotors with a Terahertz Electric Field — ●RAYMOND DEAN ASTUMIAN — Dept. of Physics, University of Maine, USA

Great progress has been made in the design and synthesis of molecular motors and rotors. Loosely inspired by biomolecular machines such as kinesin and the FoF1 ATPsynthase, these molecules are hoped to provide elements for construction of more elaborate structures that can carry out tasks at the nanoscale corresponding to the tasks accomplished by elementary machines in the macroscopic world. Most of the molecular motors synthesized to date suffer from the drawback that they operate relatively slowly (less than kHz). Here we show by molecular dynamics studies of a diethyl sulfide rotor on a gold(111) surface that a high-frequency oscillating electric field normal to the surface can drive directed rotation at GHz frequencies. The maximum directed rotation rate is 1010 rotations per second, significantly faster than the rotation of previously reported directional molecular rotors. Understanding the fundamental basis of directed motion of surface rotors is essential for the further development of efficient externally driven artificial rotors. Our results represent a step toward the design of a surface-bound molecular rotary motor with a tunable rotation frequency and direction.

Invited Talk CPP 30.5 Wed 11:45 HSZ 02
Unidirectional motion by inelastic electron tunneling — ●KARL-HEINZ ERNST — Empa, Swiss Federal Laboratories for Materials Science and Technology — Department of Chemistry, University of Zurich

Propelling single molecules in a controlled manner along an unmodified surface remains extremely challenging because it requires molecules that can use light, chemical or electrical energy to modulate their interaction with the surface in a way that generates motion. Biomolecular motors, such as the protein kinesin or the F1-ATPase, function as linear walkers or rotary motors. Chemists strive for synthesis of molecules that can perform unidirectional motion on surfaces. One successful approach was the use of ratchet-style unidirectional rotors based on overcrowded helical systems.

We show that excitation with inelastically tunneling electrons emanating from the tip of a scanning tunneling microscope (STM) very efficiently excites the rotors and leads to linear movement of the molecule on the surface for the right isomer. This requires a transient electron attachment into the LUMO, while vibronic excitation of the motor axes lead to reversible rearrangement without movement. We will discuss possible mechanisms and implication for further research and design of nanotechnological devices.

CPP 31: Focused Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale IV (original: O, joined by CPP)

Time: Wednesday 10:30–13:15

Location: TRE Ma

Topical Talk CPP 31.1 Wed 10:30 TRE Ma
From Rydberg Crystals to Bound Magnons - Probing the Non-Equilibrium Dynamics of Ultracold Atoms in Optical Lattices — ●IMMANUEL BLOCH — Max-Planck Institut für Quantenoptik, Garching, Germany — Ludwig-Maximilians-Universität, Munich, Germany

Ultracold atoms in optical lattice form an ideal testbed to probe the non-equilibrium dynamics of quantum many-body systems. In particular recent high-resolution imaging and control techniques allow to probe dynamically evolving non-local correlations in an unprecedented way. As an example, I will focus in my talk on the dynamical excitation of spatially ordered Rydberg structures that are formed through laser excitation from ground state Mott insulating atoms. In addition, I will show how single-spin and spin-pair impurities can be used to directly reveal polaron dynamics in a strongly interacting superfluid or the bound state of two magnons in a Heisenberg ferromagnet - a problem discussed first theoretically more than 80 years ago by H.A. Bethe. New atom interferometric schemes to directly probe the Green's function of a many-body system through the impurity dynamics will be discussed.

CPP 31.2 Wed 11:00 TRE Ma
Correlated Light-Matter Interactions in Cavity QED — ●JOHANNES FLICK¹, HEIKO APPEL¹, and ANGEL RUBIO^{1,2} — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — ²NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

In the electronic structure community, the quantized nature of the electrons is usually (approximately) incorporated, whereas the electromagnetic field is mostly treated classically. In contrast, in quantum optics, matter is typically simplified to models with a few levels, while the quantized nature of light is fully explored. In this work, we aim at treating both, matter and light, on an equal quantized footing.

We present exact solutions for fully quantized prototype systems consisting of atoms or molecules placed in optical one- or two-dimensional high-Q cavities and coupled to the quantized electromagnetic modes in the dipole or quadrupole coupling regime. We focus on spontaneous emission, strong-coupling phenomena, dipole-dipole couplings including van-der-Waals interactions, and Förster resonance energy transfer (FRET), all beyond the rotating-wave approximation.

This work has implications for a future development of a time-dependent density functional theory formulation of QED [1,2] for correlated multi-photon configurations.

[1] M. Ruggenthaler, F. Mackenroth, and D. Bauer, Phys. Rev. A **84**, 042107 (2011).

[2] I. Tolkatly, Phys. Rev. Lett. **110**, 233001 (2013).

CPP 31.3 Wed 11:15 TRE Ma
Optimized effective potential approach to time-dependent density functional theory for many-electron systems interacting with cavity photons — ●CAMILLA PELLEGRINI¹, JOHANNES FLICK², HEIKO APPEL², ILYA V. TOKATLY^{1,3}, and ANGEL RUBIO^{1,2} — ¹Nano-bio Spectroscopy Group and ETSF Scientific Development Centre, Departamento de Física de Materiales, Universidad del País Vasco UPV/EHU, E-20018 San Sebastián, Spain — ²Fritz-Haber Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany — ³IKERBASQUE, Bilbao, Spain

In a recent paper [1] time dependent density functional theory has been generalized to many-electron systems strongly coupled to quantum electromagnetic modes of a microcavity. Here we construct an approximation for the corresponding exchange-correlation (xc) potential by extending the optimized effective potential (OEP) method to the electron-photon system. The derivation of the OEP equation employing the non-equilibrium Green's function formalism, and the first order approximation for the electronic self-energy is presented. Beyond the mean field level, the electron-photon coupling generates a time non-local photon-mediated interaction between the electrons, whose propagator enters the exchange-like diagram. We further show the approximated xc-potential for a model two-level diatomic molecule with one electron coupled to photon modes. The comparison between the

obtained results and the exact numerical ones in the different coupling regimes (from weak up to ultra-strong) is discussed. [1] I.V. Tokatly, Phys. Rev. Lett. **110**, 233001(2013)

CPP 31.4 Wed 11:30 TRE Ma
Correlated photon-electron wavefunctions in cavity Quantum Electrodynamics — ●HEIKO APPEL¹, JOHANNES FLICK¹, RENE JESTAEDT¹, and ANGEL RUBIO^{1,2} — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — ²NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

Experimental progress in recent years has enabled the fabrication of Fabry-Perot resonators with high optical quality factors (high-Q). Such cavities allow to study the interaction of matter with a quantized light field at the single-photon level (Nobel prize 2012). In this talk we present the real-time evolution of correlated photon-electron wavefunctions in optical one- and two-dimensional high-Q cavities. We discuss implications for a multi-component density functional theory for Quantum Electrodynamics [1,2] based on the time-dependent electron density and the photon energy density.

[1] M. Ruggenthaler, F. Mackenroth, and D. Bauer, Phys. Rev. A **84**, 042107 (2011).

[2] I. Tolkatly, Phys. Rev. Lett. **110**, 233001 (2013).

CPP 31.5 Wed 11:45 TRE Ma
Photoelectron driven plasmaron excitations in (2x2)K/Graphite — ●BO HELLSING — Department of Physics, Gothenburg University, Sweden

A new type of plasmarons formed by the compound of photoelectrons and acoustic surface plasmon (ASP) excitations is investigated in the system p(2 × 2)-K/Graphite. The physics behind these types of plasmarons, e-plasmarons, is different from the ones recently found in graphene and quantum well systems, where the loss features results from the photohole-plasmon interaction in the material, h-plasmarons. Based on the first principles scheme, Time dependent density functional (TDDFT), we calculated the linear response due to the presence of the escaping photo-electron and determine the ASP dispersion. The coupling between the photoelectron and the ASP gives rise to excitation of the e-plasmarons manifested by a broad dispersive feature shifted about 0.5 eV below parabolic K induced quantum well band (QWB) in agreement with the ARPES experiment by Agdal et al. The e-plasmarons should be considered as a source of the loss satellite structure in ARPES for 2D systems. In addition they are important to take into account in theoretical studies of different compounds as they reflect an additional channel for excitations of plasmons. This could then increase the photon-plasmon conversion yield which obviously is of interest in the field of plasmonics.

CPP 31.6 Wed 12:00 TRE Ma
Charge-transfer excitations in organic systems from many-body perturbation theory — ●XAVIER BLASE¹, CARINA FABER^{1,2}, PAUL BOULANGER¹, CLAUDIO ATTACALITE¹, and IVAN DUCHEMIN² — ¹Institut Néel, CNRS and UJF, Grenoble, France — ²L.SIM/INAC, CEA, Grenoble, France

Charge-transfer excitations in organic systems lies at the heart of a large variety of physical phenomena, from photosynthesis to photovoltaics, photocatalysis or DNA denaturation. From a theoretical point of view, such nonlocal excitations are well known to lead to difficulties within the TDDFT framework, leading to the development of range-separated hybrids. We present here the merits of the Bethe-Salpeter formalism and demonstrate its ability to reproduce *cold* and *hot* Frenkel or charge-transfer excitations with remarkable accuracy [1-3]. Our calculations are based on a recent Gaussian basis implementation of the GW and Bethe-Salpeter formalism, the Fiesta initiative [1-4], allowing all-electron or pseudopotential excited states calculations for systems comprising several hundred atoms. Recent developments towards discrete and continuous embedding techniques within the many-body perturbation framework will be presented.

References: [1] C. Faber, I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. B, **86**, 155315 (2012). [2] I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. Lett. **109**, 167801 (2012). [3] I. Duchemin and X. Blase,

Phys. Rev. B 87, 245412 (2013). [4] X. Blase, C. Attaccalite, V. Olevano, Phys. Rev. B 83, 115103 (2011).

CPP 31.7 Wed 12:15 TRE Ma

Charge transfer from first principles: self-consistent GW applied to donor-acceptor systems — ●FABIO CARUSO^{1,2}, VIKTOR ATALLA¹, ANGEL RUBIO^{1,3}, MATTHIAS SCHEFFLER¹, and PATRICK RINKE¹ — ¹Fritz Haber Institute, Berlin, Germany — ²University of Oxford, UK — ³Universidad del País Vasco, San Sebastián, Spain

Charge transfer in donor-acceptor systems (DAS) is determined by the relative alignment between the frontier orbitals of the donor and the acceptor. Semi-local approximations to density functional theory (DFT) may give a qualitatively wrong level alignment in DAS, if the ionisation potential of one molecule erroneously ends up above the electron affinity of the other. An unphysical fractional electron transfer will then result in weakly interacting DAS [1]. GW calculations based on first-order perturbation theory (G_0W_0) correct the level alignment. However, the ground state is unaffected by the G_0W_0 approach, and the charge-transfer properties remain on the level of the initial DFT calculation [1]. We demonstrate that self-consistent GW (scGW) – based on the iterative solution of the Dyson's equation – provides an ideal framework for the description of charge transfer in DAS. The scGW level alignment is in agreement with experimental reference data. In addition ground- and excited-state properties are described at the same level of theory. As a result, the electron density in DAS is consistent with the level alignment between donor and acceptor, leading to a qualitatively correct description of charge-transfer properties.

[1] V. Atalla, M. Yoon, F. Caruso, P. Rinke, and M. Scheffler, Phys. Rev. B 88, 165122 (2013).

CPP 31.8 Wed 12:30 TRE Ma

What Koopmans' compliant orbital-density dependent functionals can do for you: a comprehensive benchmark of the G2-set — ●GIOVANNI BORCHI¹, NGOC LINH NGUYEN¹, ANDREA FERRETTI², ISMAILA DABO³, and NICOLA MARZARI¹ — ¹École Polytechnique Fédérale de Lausanne, Lausanne (VD), CH — ²Centro S3, CNR-NANO, Modena, IT — ³Department of Materials Science and Engineering, Penn State University, University Park (PA), USA

In this talk we present the results of benchmark calculations of the structure and electronic-structure of all molecules in the g2 set, using different flavours for Koopmans' compliant (KC) functionals. Results are compared not only to LDA and PBE, but also to orbital-density dependent calculations with the Perdew-Zunger self-interaction correction.

Our results assess the accuracy of Koopmans' compliant functionals in improving semilocal functionals to predict electronic eigenvalues and in particular ionization energies, with an accuracy that for molecules seems to be comparable or superior to that of many-body (GW) approaches. We also highlight how the Koopmans' condition tends to preserve the potential energy surface of the underlying functional, with higher reliability than e.g. PBE in structural predictions, while also providing good estimates of atomization energies.

The talk will also provide a general introduction to the theory of Koopmans' compliant functionals and their implementation in existing electronic structure codes.

Ref. Dabo *et al.*, PRB 82, 115121 (2010), and Psik highlight (2012).

CPP 31.9 Wed 12:45 TRE Ma

The electronic structure of quinacridone: Optimally tuned range-separated hybrid functional versus GW results — DANIEL LÜFTNER¹, SIVAN REFAELY-ABRAMSON², MICHAEL PACHLER¹, MICHAEL G. RAMSEY¹, LEEOR KRONIK², and ●PETER PUSCHNIG¹ — ¹Institut für Physik, Karl-Franzens-Universität Graz, Austria — ²Department of Materials and Interfaces, Weizmann Institute of Science, Israel

Quinacridone is an organic molecule (C₂₀H₁₂N₂O₂) utilized in the formation of organic pigments. It has also been discussed for usage in organic electronics particularly due to its stability under ambient conditions and its tendency to form self-assembled supramolecular networks. Here, we report on its electronic structure, both, for the isolated molecule as well as for the alpha- and beta- bulk molecular crystal polymorphs. We employ an optimally tuned range-separated hybrid functional (OT-RSH) within density functional theory as well as GW corrections within a many-body perturbation theory framework. A comparison of the theoretical results obtained with the different levels of theory and a subsequent comparison with experimental data from angle-resolved photoemission spectroscopy emphasize the need for going beyond simple semi-local DFT-functionals in order to obtain the correct orbital ordering. Furthermore the comparison indicates that the results obtained with OT-RSH greatly improve those of standard DFT functionals and achieve an agreement with experiment at the level of GW calculations, thus making the OT-RSH an alternative to the computationally more expensive GW approach.

CPP 31.10 Wed 13:00 TRE Ma

GW many-body perturbation theory for electron-phonon coupling calculations — ●CARINA FABER^{1,2}, PAUL BOULANGER¹, IVAN DUCHEMIN^{1,2}, and XAVIER BLASE¹ — ¹Institut Néel, CNRS, Grenoble, France — ²INAC, CEA, Grenoble, France

We study within many-body perturbation theory the electron-phonon coupling in organic systems, taking as paradigmatic examples the fullerene molecule and the pentacene crystal [1,2]. We show that the strength of the electron-phonon coupling potential is dramatically underestimated at the LDA level, while GW calculations offer an excellent agreement with experiments [1]. Further, combining GW calculations of the electronic band structure and of the electron-phonon coupling in crystalline pentacene, we show that the hole bands dispersion can be reconciled with photoemission experiments, by solving non-perturbatively (DMFT) the effect of electron-phonon coupling on the electronic self-energy [2]. We finally explore various approximations that may allow to combine the GW formalism with convenient linear response formalisms beyond the frozen-phonon techniques. Our calculations are performed with the Fiesta package, a Gaussian based GW and Bethe-Salpeter code allowing all-electron or pseudopotential calculations with various resolution of the identity techniques and without any plasmon pole approximation [3,4].

[1] C. Faber *et al.*, Phys. Rev. B 84, 155104 (2011) [2] S. Ciuchi *et al.*, Phys. Rev. Lett. 108, 256401 (2012) [3] C. Faber, I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. B, 86, 155315 (2012). [4] I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. Lett. 109, 167801 (2012).

CPP 32: Glasses (original: DF, joined by CPP, DY)

Time: Wednesday 11:45–12:45

Location: WIL B321

CPP 32.1 Wed 11:45 WIL B321

Two-level tunneling systems in amorphous alumina — ALEJANDRO P. PAZ¹, IRINA V. LEBEDEVVA¹, ILYA V. TOKATLY^{1,2}, and ANGEL RUBIO^{1,3,4} — ¹Nano-bio Spectroscopy Group, Universidad del País Vasco, San Sebastian, Spain — ²IKERBASQUE, Bilbao, Spain — ³Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — ⁴European Theoretical Spectroscopy Facility

The decades of research on thermal properties of amorphous solids at temperatures below 1 K suggest that their anomalous behaviour can be related to quantum mechanical tunneling of atoms between two nearly equivalent states that can be described as a two-level system (TLS) [1]. This theory is also supported by recent studies on microwave spectroscopy of superconducting qubits [1]. However, the microscopic nature of TLSs remains unknown. To identify bistable structural motifs in amorphous alumina we have performed extensive classical molecular dynamics simulations. Several motifs with only one or two atoms jumping by considerable distance ~ 0.5 Å were found at temperature 25 K. Accounting for the surrounding environment relaxation was shown to be important up to distances ~ 7 Å. The energy asymmetry and barrier for the detected motifs lied in the ranges 0.5 - 2 meV and 4 - 15 meV, respectively, while their density was about 1 motif per 10000 atoms. Tuning of motif asymmetry by strain was demonstrated with the coupling coefficient below 1 eV. The tunnel splitting for the symmetrized motifs was estimated on the order of 0.1 meV. The properties of the discovered motifs are in good agreement with the available experimental data. [1] G. J. Grabovskij et al. Science 338, 232 (2012).

CPP 32.2 Wed 12:05 WIL B321

Resistive Properties of Lithium-Ion Conducting LiSICON Glass Ceramics in Contact with Lithium Metal and Nonaqueous Electrolytes — KIM OLIVER HOFMANN^{1,2}, MEIKE SCHNEIDER², MARIA-LOUISA REICH², MIRIAM KUNZE², and MICHAEL VOGEL¹ — ¹Institut für Festkörperphysik, Technische Universität Darmstadt — ²Schott AG Mainz

Lithium-ion conducting glass ceramics with LiSICON type crystalline phase are promising materials as solid electrolytes in future batteries due to their high ionic conductivity, which is higher than 1×10^{-5} S/cm.

These materials can not only be applied to solid state lithium batteries but also for lithium-sulfur and lithium-air batteries. For these applications the LiSICON materials need to be stable against metallic Li and battery specific liquid electrolytes.

Lithium contact stability is derived by measuring the impedance Z over a period of seven days. In case the glass ceramic reacts with metallic lithium and reduces the polyvalent ions in the glass ceramic like Ge or Ti, the impedance Z is increasing and the sample turns black, noticeably. Further on the impedance spectroscopy is used to determine the interaction of glass ceramics with different liquid electrolytes. The impedance spectra are additionally analyzed by a distribution of relaxation times, based on a distribution function over infinite serial connected RC elements [1]. The resistance contribution of the glass ceramics in contact with liquid electrolytes can be distinguished in interface, grain boundary and grain core resistance by this method.

[1] H. Schichlein et al., J. Appl. Electrochem., 32 (2002) 875- 882

CPP 32.3 Wed 12:25 WIL B321

Optical properties of trivalent rare-earth ions in barium borate glasses — SEBASTIAN LOOS¹, FRANZISKA STEUDEL², BERND AHRENS^{1,2}, and STEFAN SCHWEIZER^{1,2} — ¹South Westphalia University of Applied Sciences, Lübecker Ring 2, 59494 Soest — ²Fraunhofer Institute for Mechanics of Materials IWM, Walter-Hülse-Str. 1, 06120 Halle (Saale)

Rare-earth doped glasses gain increasing importance in optical devices, such as fibre lasers or light emitting diodes. Luminescence properties of rare-earth ions are well-known, but absolute photoluminescence quantum efficiencies have been insufficiently studied. In this work, series of Sm^{3+} , Eu^{3+} , and Tb^{3+} doped barium borate glasses are investigated for their potential application as frequency down-converters in solid state lighting and photovoltaics. Photoluminescence quantum efficiencies have been analyzed for rare-earth doping levels up to 5 at.%. The best values of more than 50% are achieved for Eu^{3+} doping. To increase the photoluminescence quantum efficiency even further, the Sm^{3+} -doped samples have been co-doped with a second rare-earth ion, namely Eu^{3+} or Tb^{3+} . Here, energy transfer processes between Sm^{3+} and the second rare-earth ion become important; they are discussed in detail.

CPP 33: Cytoskeleton (original: BP, joined by CPP)

Time: Wednesday 9:30–13:00

Location: HÜL 386

Topical Talk

CPP 33.1 Wed 9:30 HÜL 386

Intermediate filaments - mechanical building blocks and dynamic elements of the cell — SARAH KÖSTER — Institut für Röntgenphysik, Georg-August-Universität Göttingen, Göttingen, Germany

Intermediate filaments (IFs) are a major component of the eukaryotic cytoskeleton. By contrast to actin filaments and microtubules, which are highly conserved throughout cell types and organisms, IFs are diverse and are believed to define cellular mechanics to a considerable degree. In the cell, IFs form complex hierarchical networks and bundles that are linked to other cytoskeletal proteins. In vitro experiments on purified proteins in combination with cell experiments thus provide insight into the mechanical and dynamic properties of IFs. Following this concept, we investigate the mechanical characteristics of individual purified IFs in confinement and inter-filament interactions mediated by multivalent cations. In the cell, bundling of IFs is more complex as various regulatory proteins are involved. Despite this complexity, direct observation of the bundle- and network-dynamics sheds light onto the mechanical and structural properties of the bundles themselves as well as of the surrounding cytoplasm.

CPP 33.2 Wed 10:00 HÜL 386

Keratin 8/18 Networks and their Interplay with Different Crosslinkers — INES MARTIN¹, TOBIAS NECKERNUSS¹, TOBIAS PAUST¹, MICHAEL BEIL², HARALD HERRMANN³, and OTHMAR MARTI¹ — ¹Department of Experimental Physics, Ulm University, Ulm, Germany — ²Clinic of Internal Medicine I, Ulm University, Ulm, Germany — ³Division of Molecular Genetics, German Cancer Research Center

(DKFZ), Heidelberg, Germany

The keratin 8/18 dimer is a structural building block of intermediate filaments (IFs), which are basic constituents of the cytoskeleton in epithelial cells. They are responsible for the stiffness of cells and responses to mechanical stimuli. The understanding of the cytoskeleton is for example important for the characterization of the movement of metastasizing cells.

Keratin filaments can be crosslinked by proteins like plectin, which also link IFs to hemidesmosomes as well as to different constituents of the cytoskeleton. Additionally Keratins can be bundled by ions like MgCl_2 or KCl . In this work we assembled keratin 8/18 together with plectin, KCl and MgCl_2 *in vitro* to form crosslinked networks. We checked the resulting networks with Scanning Electron Microscopy (SEM) and Immuno-Gold-Labeling. With this we were able to identify the position of plectin molecules. The viscoelastic network properties were measured by passive microrheology and we compared *in vitro* assembled networks without crosslinker and with KCl , MgCl_2 and plectin.

CPP 33.3 Wed 10:15 HÜL 386

The role of keratins for the mechanical properties of keratinocytes — GLORIA FABRIS¹, RONALD SPRINGER¹, LENA RAMMS¹, REINHARD WINDOFFER², NICOLE SCHWARZ², SIMONE STIEFEL¹, NILS HERSCH¹, THOMAS MAGIN³, RUDOLF LEUBE², BERND HOFFMANN¹, and RUDOLF MERKEL¹ — ¹ICS-7, Forschungszentrum Jülich, Germany — ²Institute of Molecular and Cellular Anatomy, RWTH Aachen, Germany — ³Translational Centre for Regenerative Medicine and Institute

of Biology, University of Leipzig, Germany

Keratin intermediate filaments contribute forming the cytoskeleton of many epithelial cell types: in keratinocytes, for example, type I and type II keratins form a stable network which is supposedly crucial to the mechanical integrity at the cellular and tissue level.

Owing to compensatory keratin expression, the overall contribution of keratin proteins to cell mechanics is difficult to examine in vivo upon deletion of single genes. In our study, we compared wild type mouse epidermal keratinocytes with mutant cells (KO) in which the whole gene cluster expressing members of the keratin family was deleted [1].

Atomic force microscopy indentation experiments showed a highly significant softening of KO keratinocytes when compared with the wild type, which could not be attributed to modifications of other cytoskeletal structures (i.e. microfilaments/microtubules).

Data clearly indicated that the keratin cytoskeleton plays a vital role in conferring stiffness and structural stability to keratinocytes.

[1] Ramms L, et al., PNAS 110(46):18513-18518 (2013).

CPP 33.4 Wed 10:30 HÜL 386

Correlations in the random hydrolysis model of actin filaments and microtubules — ●THOMAS NIEDERMAYER and REINHARD LIPOWSKY — Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

The polymerization (assembly) and depolymerization (disassembly) of actin filaments and microtubules are pivotal for cell motility, cell adhesion, and cell division. These dynamic processes are controlled by analogous mechanisms: Actin monomers can bind ATP or ADP, whereas tubulin dimers bind either GTP or GDP. In both cases, the hydrolysis of the bound ATP/GTP within the filaments increases the subunit dissociation rate and thereby couples to the stochastic dynamics of filament growth and shrinkage. In the widely discussed random hydrolysis model, which appropriately describes actin and microtubule dynamics in vitro, the hydrolysis rate is identical at each filament subunit. We studied this model by a novel theoretical approach and stochastic simulations. While mean field solutions, which are considered in the recent literature, fail to describe the filament dynamics in physiologically relevant cases, our analytical approach matches the simulations, as it accounts for correlation effects.

CPP 33.5 Wed 10:45 HÜL 386

Nematic microstructure in biopolymer solutions — ●MARC LÄMMEL and KLAUS KROY — Institut für Theoretische Physik, Leipzig, Germany

Alignment of polymers is a major mechanism employed by cells to adapt their mechanical strength. Since it is easily induced by steric and energetic interactions, as well as by shear ordering, it is also ubiquitous in biopolymer solutions and gels. Here, we address the influence of such nematic order on the packing structure of semiflexible polymer networks, based on the wormlike chain model. The complicated many-body problem is approached utilizing the concept of the tube [1], which accounts for caging of a test polymer by surrounding filaments. As recently elucidated [2], this cage, rather than being homogeneous, features characteristic variations along the polymer contour. In our approach, the tube is represented through of harmonic confinement potential that is self-consistently determined. In particular, we analyze the effect of local nematic order on the microstructure in terms of the mean tube radius and its distribution [3], for which we observe a remarkable agreement between the analytical predictions and results of hybrid Brownian dynamics/Monte Carlo simulations [4].

[1] Morse, Phys. Rev. E 63, 031502 (2001)

[2] Glaser and Kroy, Phys. Rev. E 84, 051801 (2011)

[3] Glaser *et al.*, Phys. Rev. Lett. 105, 037801 (2010)

[4] Ramanathana and Morse, J. Chem. Phys. 126, 094906 (2007)

CPP 33.6 Wed 11:00 HÜL 386

Elasto-plastic response of reversibly crosslinked biopolymer bundles — ●POULOMI SADHUKHAN and CLAUS HEUSSINGER — Institute for theoretical Physics, University of Goettingen, Friedrich Hund Platz 1, 37077 Goettingen, Germany.

We model cytoskeletal actin bundles under stress in order to explain the elasto-plastic response observed in recent experiments (D. Strehle *et al* 2011). In doing so, we allow crosslinks to reversibly un- and rebound to the actin filaments. Cross-link reorganization leads to defect formation, which we speculate to be the underlying mechanism responsible for the residual ("plastic") deformation observed in the experiments.

The problem is studied for two cases related by the Legendre transformation - under given force and under given deflection of the bundle. Our main result is in agreement with the experiment. We show that a small bending stress can deform the bundle for soft crosslinks, and shows plastic-like behaviour. On the other hand, bundles with stiff crosslinks show elastic behaviour. Along with this, we also observe how the defect position is related to the applied stress and crosslink stiffness and how the required stress to create a residual deformation of the bundle varies with the crosslink stiffness.

15 min. break

CPP 33.7 Wed 11:30 HÜL 386

Physical basis of spindle self-organization — ●JAN BRUGUES¹ and DANIEL NEEDLEMAN² — ¹MPI for Physics of Complex Systems/MPI of the Molecular Cell Biology and Genetics, Dresden, Germany — ²Center for Systems Biology, Harvard University, Cambridge, USA

The spindle, which segregates chromosomes during cell division, is known to be composed of microtubules and hundreds of other proteins, but the manner in which these molecular constituents self-organize to form the spindle remains unclear. Here we use a holistic approach, based on quantitative measurements in spindles of the spatio-temporal correlation functions of microtubule density, orientation and stresses, to identify the key processes responsible for spindle self-organization. We show that microtubule turnover and the collective effects of local microtubule interactions, mediated via motor proteins and crosslinkers, can quantitatively account for the dynamics and the structure of the spindle. We thus reveal the physical basis of spindle self-organization and provide a framework that may be more generally useful for understanding cytoskeletal function in vivo.

CPP 33.8 Wed 11:45 HÜL 386

Structural and mechanical properties of the kinetochore: a biophysical approach. — ●GHEORGHE COJOC¹, EMANUELE ROSCIOLI², LIJUAN ZHANG³, IVA M. TOLIĆ-NØRRELYKKE¹, DANIELA CIMINI², and JURAJ GREGAN³ — ¹Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — ²Dept. Biological Sciences, Virginia Tech, Blacksburg, VA, USA — ³Max F. Perutz Laboratories, University of Vienna, Vienna, Austria

The equal partitioning of replicated sister chromatids during cell division depends on proper attachment of kinetochores (KTs) to the microtubules (MTs) emanating from opposite poles. The KT is a multidomain structure that assembles during mitosis to create the MT-binding sites on the centromere. Although mounting evidence suggests that the mechanical properties of KT may contribute to faithful chromosome segregation, an in-depth characterization of such properties is still lacking. Here, we used merotelic KT as a model to characterize the mechanical properties of different KT subdomains. Merotelic KT attachment is an error in which MTs nucleating from both poles attach to the same KT. Merotelic KT persisting into anaphase become significantly stretched, which makes them an ideal model to study KT mechanical properties. We developed an in vivo assay to investigate KT mechanics by releasing the forces acting on the merotelic KT and performing live cell imaging at high spatial and temporal resolution. In our assay, the forces on the KT are released by severing (using laser microsurgery) one of the two MT bundles attached to the stretched merotelic KT.

CPP 33.9 Wed 12:00 HÜL 386

Network elasticity of microtubules cross-linked with ds DNA — ●MEENAKSHI PRABHUNE¹, KNUT HEIDEMANN², MAX WARDETZKY², CHRISTOPH F. SCHMIDT¹, and FLORIAN REHFELDT¹ — ¹Third Institute of Physics-Biophysics, Georg August University, Göttingen — ²Department for Numerical and Applied Mathematics, Georg August University, Göttingen

The cytoskeleton is a composite polymer network of cytoskeletal filaments ranging from rod-like microtubules and actin bundles to softer semi-flexible intermediate filaments and actin filaments. Studying the interactions between these heterogeneous filaments is an important step in understanding cell mechanics. Single-component in vitro networks have been studied, but well defined composites are more difficult to construct and are not yet well understood. Here, we have generated heterogeneous networks in vitro by cross-linking microtubules using ds DNA via a hetero-bifunctional cross-linker (sulpho SMCC). DNA as a cross-linker has the unique advantage of having a monodisperse

well-defined length, which we vary in our experiments. We have measured the linear and nonlinear shear-elastic response in these networks by microrheology experiments. Simultaneously, we also compare the experimental data to numerical simulations that we have developed for networks of stiff slender rods connected by semi-flexible linkers.

CPP 33.10 Wed 12:15 HÜL 386

Fluorescent beads disintegrate actin networks — ●TOM GOLDE, CARSTEN SCHULDT, JÖRG SCHNAUSS, DAN STREHLE, MARTIN GLASER, and JOSEF KÄS — Institut für Experimentalphysik 1, Universität Leipzig, Leipzig, Deutschland

We studied the influence of fluorescent polystyrene beads on both entangled and cross-linked actin networks. Thermal bead fluctuations were observed via video particle tracking and analyzed with one-point microrheology. Illumination of fluorescent beads with their appropriate excitation wavelength leads to a drastic softening of actin gels. Other wavelengths and bright field microscopy do not increase thermal bead fluctuations. This effect cannot be significantly reduced by adding common oxygen scavengers. We conclude that the usage of fluorescent beads impairs results when studying the microrheology of actin networks [1].

[1] Golde et al., Physical Review E 88, 044601 (2013)

CPP 33.11 Wed 12:30 HÜL 386

Circular Dorsal Ruffles — ●ERIK BERNITT and HANS-GÜNTHER DÖBEREINER — Institut für Biophysik, Universität Bremen, 28334 Bremen

Circular Dorsal Ruffles (CDRs) are actin-based structures that form at the dorsal side of adherent cells like, e.g., fibroblasts. CDRs are usually of a ring-like morphology and exhibit a soliton-like propagation. We are interested in the underlying mechanism that leads to CDR formation and propagation. We observe a rich set of phenomena that allows to draw conclusions on the underlying processes. Among them are periodic formations of CDRs at the same location, fusion and

fission dynamics, stationary behavior, and reflection of CDRs.

Apparently, cell morphology plays a key role for CDR dynamics. Despite the typically inhomogeneous shape of adherent fibroblasts we find a universal trajectory in phase space that seems to govern CDR dynamics.

To simplify the constraints set by the morphology, we plate cells on circular fibronectin patterns. This system allows us to compare data acquired on different cells. We find waves that propagate in angular direction with a remarkably conserved velocity.

CPP 33.12 Wed 12:45 HÜL 386

FtsZ rings and helices: physical mechanisms for the dynamic alignment of biopolymers in rod-shaped bacteria — ●ELISABETH FISCHER-FRIEDRICH, BENJAMIN M. FRIEDRICH, and NIR S. GOV — Weizmann Institute of Science, Rehovot, Israel

In many bacterial species, the protein FtsZ forms a cytoskeletal ring that marks the future division site and scaffolds the division machinery. In rod-shaped bacteria, most frequently membrane-attached FtsZ rings or ring fragments are reported and occasionally helices. By contrast, axial FtsZ clusters have never been reported. In this paper, we investigate theoretically how dynamic FtsZ aggregates align in rod-shaped bacteria. We study systematically different physical mechanisms that affect the alignment of FtsZ polymers using a computational model that relies on autocatalytic aggregation of FtsZ filaments at the membrane. Our study identifies a general tool kit of physical and geometrical mechanisms by which rod-shaped cells align biopolymer aggregates. Our analysis compares the relative impact of each mechanism on the circumferential alignment of FtsZ as observed in rod-shaped bacteria. We determine spontaneous curvature of FtsZ polymers and axial confinement of FtsZ on the membrane as the strongest factors. Including Min oscillations in our model, we find that these stabilize axial and helical clusters on short time scales, but promote the formation of an FtsZ ring at the cell middle at longer times. This effect could provide an explanation to the long standing puzzle of transiently observed oscillating FtsZ helices in *Escherichia coli* cells prior to cell division.

CPP 34: Organic Electronics and Photovoltaics (joint session with DS/HL/O) IV

Spectroscopy, OFETs, OLEDs, Photo switches

Time: Wednesday 15:00–18:15

Location: ZEU 260

CPP 34.1 Wed 15:00 ZEU 260

Comprehensive efficiency analysis of organic light-emitting diodes featuring horizontal emitter orientation and triplet-to-singlet up-conversion — ●TOBIAS SCHMIDT¹, BERT SCHOLZ¹, CHRISTIAN MAYR¹, ANDREAS RAUSCH², THOMAS WEHLUS², DIRK MICHAELIS³, NORBERT DANZ³, THILO REUSCH², 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 external quantum efficiency (EQE) of an organic light-emitting diode can strongly be affected by orientation of the emissive dipole moments, and for fluorescent dyes, by triplet-to-singlet up-conversion leading to an enhanced radiative exciton fraction (η_r), exceeding the spin-statistical limit of 25%. By a combination of EQE investigations with time resolved photo- and electroluminescence measurements we are able to quantify the lower limit of the additionally created singlet excitons, e.g. by thermally activated delayed fluorescence, as well as the factors being responsible for light-outcoupling. For the investigated fluorescent system the EQE is boosted by two effects. First, due to horizontal alignment of the transition dipole moments, the outcoupling factor is enhanced by a factor of 1.3. Second, the enhanced η_r value of 36%, results in an additional efficiency increase by a factor of 1.44. As a consequence of the combination of both effects the EQE almost doubles and values up to 5% are achieved for direct emission in spite of a comparatively low emitter efficiency of 40% only.

CPP 34.2 Wed 15:15 ZEU 260

Multi-analytical investigation of SAM formation in printing relevant timescales III: OFET devices — ●MILAN ALT^{1,2,6}, JANUSZ SCHINKE^{2,3}, SABINA HILLEBRANDT^{2,5}, MARC HÄNSEL^{2,4}, KAJA DEING^{2,6}, ULI LEMMER^{1,2}, and NORMAN MECHAU^{1,2} — ¹Karlsruher Institute of Technology — ²InnovationLab, Heidelberg — ³TU Braun-

schweig — ⁴TU Darmstadt — ⁵Uni Heidelberg — ⁶Merck KGaA

Self-assembled monolayers (SAMs) can be used to effectively reduce contact resistances originating from energetic misalignments at metal-semiconductor interfaces. Solution processing of SAMs has been intensively studied and is in principle compatible with high throughput printing techniques. However, most studies on SAMs feature immersion in very dilute solutions for many hours, in some cases up to several days. The objective of this work is to understand SAM accumulation with a focus on short time scales in order to estimate whether the deposition of well performing SAMs can be speeded up sufficiently to be compatible with typical film drying times in printing. We combined analytical characterization of SAM treated metal surfaces via photoelectron- and IR-spectroscopy, as well as Kelvin Probe with measurements of the actual injection barriers in OFET devices. We chose the widely used 1H,1H,2H,2H-Perfluorodecanethiol SAM and investigated its quality and charge injection performance in dependency of the process parameters immersion time and molecular concentration. Additionally, we studied the impact of ambient condition on SAM deposition and the resulting SAM performance, in order to account for a realistic fabrication environment.

CPP 34.3 Wed 15:30 ZEU 260

Multi-analytical investigation of SAM formation on printing-relevant time scales I: Kelvin probe and photoelectron spectroscopy — ●JANUSZ SCHINKE^{1,5}, MARC HÄNSEL^{2,5}, MILAN ALT^{3,4,5}, SABINA HILLEBRANDT^{2,5}, ERIC MANKEL^{6,5}, WOLFRAM JAEGERMANN^{6,5}, WOLFGANG KOWALSKY^{1,5}, and ROBERT LOVRINCIC^{1,5} — ¹TUBS, Inst. f. Hochfrequenztechnik — ²Uni HD, Kirchhoff-Inst. für Physik — ³Karlsruher Inst. f. Technologie — ⁴Merck KGaA — ⁵InnovationLab GmbH, Heidelberg — ⁶TUD, Materials Science Inst.

In organic electronic devices, charge injection at the contacts is crucial for electrical performance. The devices require electrodes with a suf-

ficiently low contact resistance at the metal-semiconductor interface to inject into or collect charge carriers from the transporting layer. A smart way to align the energetics at the interface is the use of self-assembled monolayers (SAMs). We have studied the properties of 1H,1H,2H,2H-Perfluorodecanethiol using photoelectron spectroscopy (XPS/UPS), infrared spectroscopy (IR), ambient Kelvin probe (KP), and contact angle (CA) measurements and the injection barriers were also measured in actual devices - organic field effect transistors. Using these methods we were able to obtain a very deep understanding of the whole SAM adsorption process, as well as the impact of immersion time, concentration and the influence of ambient conditions on the resulting monolayer and its performance. With this knowledge we estimate optimized parameters to speed up the treatment process, in contrast to most studies where long immersion times are used, to be compatible with typical times used in standard printing methods.

CPP 34.4 Wed 15:45 ZEU 260

Multi-analytical investigation of SAM formation on printing-relevant time scales II: infrared-reflection-absorption-spectroscopy — ●SABINA HILLEBRANDT^{1,5}, JANUSZ SCHINKE^{2,5}, MILAN ALT^{3,4,5}, ROBERT LOVRINCIC^{2,5}, TOBIAS GLASER^{1,5}, and AN-NEMARIE PUCCI^{1,5} — ¹Universität Heidelberg, Kirchhoff-Institut für Physik — ²Technische Universität Braunschweig, Institut für Hochfrequenztechnik — ³Karlsruher Institut für Technologie — ⁴Merck KGaA, Darmstadt — ⁵Innovationlab GmbH, Heidelberg

In organic semiconductor devices the improvement of charge carrier injection between metal contact and organic semiconductor is a major concern. Self-assembled monolayers (SAMs) built up interface dipoles on metal surfaces that can increase or lower the work function of the material. Therefore SAMs can be used as injection layers. The properties of solution-processed SAMs such as orientation and interface dipole are influenced by various factors like concentration of the molecule in solution, immersion time and purity of the solution or substrate.

Infrared-reflection-absorption-spectroscopy (IRRAS) is very sensitive to changes in the orientation of SAMs on metal surfaces, thus we performed IRRAS measurements on SAMs consisting of 1H,1H,2H,2H-perfluorinated decanethiol on evaporated gold substrates. Orientation, ordering and quality of the SAM were investigated under systematic variation of immersion time and concentration of the molecule in solution. Taking into account realistic printing conditions we also investigated very short immersion times and high concentrations as well as the impact of oxygen in solvent and substrate on the layer formation.

CPP 34.5 Wed 16:00 ZEU 260

Towards fully printed organic light-emitting diodes: investigation of solution processed electron injection layers — ●SEBASTIAN STOLZ^{1,4}, GERARDO HERNANDEZ-SOSA^{1,4}, MICHAEL SCHERER^{2,4}, ERIC MANKEL^{3,4}, ROBERT LOVRINCIC^{2,4}, JANUSZ SCHINKE^{2,4}, ULI LEMMER^{1,4}, and NORMAN MECHAU^{1,4} — ¹Karlsruhe Institute of Technology, Light Technology Institute — ²Technische Universität Braunschweig, Institut für Hochfrequenztechnik — ³Technische Universität Darmstadt, Materials Science Institute, Surface Science Division — ⁴InnovationLab GmbH, Heidelberg

The fabrication of organic light-emitting diodes (OLEDs) by high throughput printing techniques requires the development of solution processable electron injection layers. Today, either alkali salts or low work-function alkaline earth metals are used as cathode layers in OLEDs. As these materials are highly reactive, they cannot be easily solution processed. In this work, we present blue fluorescent light-emitting diodes which use silver in combination with Polyethylenimine (PEI) and Polyethylenimine-ethoxylated (PEIE) as cathode layer. We demonstrate that both materials can be effectively used as electron injection layers in OLEDs and correlate the performance of the devices to the characteristics of the PEI(E) layers. Photoelectron spectroscopy is used to estimate the polymer thickness and the corresponding change in cathode work-function while the homogeneity of the layers is evaluated by AFM measurements. We show that OLEDs using PEI/PEIE and silver as cathode layer yield an improved performance and shelf lifetime compared to reference devices that use calcium, instead.

15 min. break

CPP 34.6 Wed 16:30 ZEU 260

Micro-structured organic field effect transistor on commercial poly(urethane) resin as substrate and gate dielectric — JAN HARTEL, DERCK SCHLETTWEIN, and ●CHRISTOPHER KEIL — Institute of Applied Physics, Laboratory of Materials Research, Justus-Liebig-

University Giessen, Germany.

Dielectric layers of a commercial cross-linked poly (urethane) (PU) were prepared on a conductively coated film and served as gate dielectric and as substrate for the growth of an organic semiconductor film in an alternative approach to all-organic field effect transistors (OFET). A method was developed to process micro-structured electrodes on top of the PU dielectric layer which proved superior to the traditional lift-off-procedure. The influence of the aspect ratio of the electrodes within the organic transistor on a given dielectric layer will be discussed with respect to the calculation of the relative permittivity and the gate capacitance. A method is proposed to compensate short electrode effects which would otherwise lead to an underestimation of the gate capacitance and hence to a miscalculation of the OFET properties.

CPP 34.7 Wed 16:45 ZEU 260

Time-resolved potentiometry of organic thin film transistors — ●JAN MURAWSKI, TOBIAS MÖNCH, MORITZ PHILIPP HEIN, PETER MILDE, and LUKAS M. ENG — Technische Universität Dresden, Institut für Angewandte Photophysik

High speed application still poses a challenge for organic thin film transistors (OTFTs) due to their low charge carrier mobilities, high driving voltages, and low on/off-current ratios. Few investigations have been reported on the switching dynamics of OTFTs on the nanoscale, even fewer in the relevant temporal operation regime as required for high speed applications. Yet, such investigations are crucial for understanding the bottle-necks in OTFTs dynamic performance.

Here, we introduce time-resolved Kelvin probe force microscopy (tr-KPFM) to track the time evolution of surface potential wave fronts inside the channel of a pentacene-based bottom-gate coplanar OTFT. The relevant dynamical evolution proceeds in the microsecond regime and is easily resolved by our quantitative tr-KPFM method. Comparing our experiment with simulations reveals the presence of Schottky barriers in the real device to be responsible not only for a reduced effective electric field across the transistor channel (and thus a reduced field mobility) but also for inducing a delayed re-injection of charge carriers at the electrode-semiconductor interface. Although the charge-carrier mobility would allow for faster switching, charging the Schottky barrier constitutes the bottle-neck to be overcome for higher working frequencies in OTFTs.

CPP 34.8 Wed 17:00 ZEU 260

High-Mobility, Low-Voltage Organic TFTs based on Air-Stable DNNT Derivatives: Time-Dependent Improvement in Contact Resistance and Dynamic Performance — ●ULRIKE KRAFT^{1,3}, UTE ZSCHIESCHANG¹, KAZUO TAKIMIYA², EDWIN WEBER³, and HAGEN KLAUK¹ — ¹Max Planck Institute for Solid State Research, Stuttgart, Germany — ²RIKEN Advanced Science Institute, Wako, Japan — ³Technical University Bergakademie Freiberg, Germany

The organic semiconductor dinaphthothienothiophene and its derivatives C10-DNNT and diphenyl-DNNT provide larger carrier mobilities and better air stability than, e.g., pentacene. We present a detailed comparison of the thin-film morphology, static and dynamic performance and stability of low-voltage (3 V) thin film transistors based on vacuum-deposited films. Freshly fabricated TFTs (channel length: 100 μm) have hole mobilities ranging from 3 cm^2/Vs (DNNT) to 5 cm^2/Vs (diphenyl-DNNT), with on/off ratios of 10^7 .

During the first few hours after fabrication, the effective mobility of short-channel TFTs ($L=1 \mu\text{m}$) increases by about 20-30%, due to an improvement in the contact resistance (measured with TLM). The dependence of this effect on the exposure to different gas atmospheres, humidity and to light was investigated. To study the impact on the dynamic performance of the TFTs, we fabricated unipolar ring oscillators on flexible PEN substrates. The stage delay of DNNT TFTs ($L=1 \mu\text{m}$) measured at 3 V drops from 920 to 410 ns during the first 4 days of exposure to ambient air, which is the shortest delay reported for flexible organic TFTs at supply voltages $<10 \text{ V}$.

CPP 34.9 Wed 17:15 ZEU 260

Continuously tunable organic semiconductor distributed Feedback (DFB) lasers as an example for optical components built from shape-memory polymers — ●SENTA SCHAUER¹, XIN LIU², TOBIAS MEIER¹, MARC SCHNEIDER¹, MATTHIAS WORGULL¹, ULI LEMMER^{1,2}, and HENDRIK HÖLSCHER¹ — ¹Karlsruhe Institute of Technology, Institute of Microstructure Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — ²Karlsruhe Institute of Technology, Light Technology Institute, En-

gesserstraße 13, 76131 Karlsruhe, Germany

Phase gratings are important tools for many applications in optics and photonics, e.g., they serve as resonators in DFB-lasers. We manufactured Bragg gratings from a shape-memory polymer (SMP) to tune their period over a wide range without any mechanical components. SMPs can remember a predefined shape and recover to it even after strong deformations, if they are triggered by a stimulus. We used the polyurethane Tecoflex(R), which is a thermally triggered SMP, to fabricate nanostructured gratings via hot embossing. After stretching, these gratings feature an increased period which shrinks back to its original length after the activation of the recovery process. In order to demonstrate the practical applicability of these gratings as useful components for photonics, we successfully fabricated continuously tunable DFB-lasers based on SMP grating substrates with Alq3:DCM serving as active material. By changing the grating period via the shape-memory effect, the emitted wavelength of the laser changes likewise. So far we demonstrated shifts of the emission spectrum by 30nm.

CPP 34.10 Wed 17:30 ZEU 260

Optical studies of excitonic precursor spin species under magnetic resonance in organic light emitting diodes. — ●HERMANN KRAUS, SEBASTIAN BANGE, and JOHN M. LUPTON — Universität Regensburg, 93040 Regensburg, Deutschland

Large magnetoresistance effects e.g. due to spin-dependent recombination rates are well-known for OLEDs [C. Boehme et al., Nat. Nano 8, 612 (2013)], although models are still under debate given that they remain hard to verify from a measurement of integrated current and luminance values [J. M. Lupton et al., Nature Mat. 7, 598 (2008)]. Spin resonance of paramagnetic species enables direct manipulation of carrier and excitonic precursor spins, providing a wealth of new insight into dynamic spin properties. Previous work on electrical or optical detection of spin manipulation [W. J. Baker et al., Nature Comm. 3, 898 (2012); W. J. Baker et al., Phys. Rev. B 84, 165205 (2011)] misses out on the opportunity to directly observe the presence of triplet exciton species that are at the heart of spin-dependent recombination models. A few polymeric and small-molecular compounds are now known to exhibit reasonable triplet emission without modification of the polaron pair and exciton dynamics by strong spin-orbit interaction [D. Chaudhuri et al., Angew. Chem. Int. Ed. DOI 10.1002/anie.201307601(2013); J. M. Lupton et al., Phys. Rev. Lett. 89 167401(2002)]. Those materials are ideal candidates to directly track spin singlet and triplet excitonic species in organic light-emitting diodes under conditions of magnetic resonance, by comparing the fluorescence (singlet) to phosphorescence (triplet) intensity.

CPP 34.11 Wed 17:45 ZEU 260

Ab-initio quantum dynamics simulation of photo-induced molecular switching: Azobenzene on coinage metals — ●REINHARD J. MAURER and KARSTEN REUTER — Department Chemie,

Technische Universität München, Germany

The constant pursuit towards further miniaturization of electronic devices slowly reaches the point where individual molecules may serve as the main functional units. Unfortunately, more often than not, an inherent molecular function is quenched by overly strong coupling to the environment; a permanent danger, specifically in the case of metal surface adsorption. Nevertheless, metal surface adsorption may also introduce new functionality, such as in the case of photo-induced molecular switching of tetra-*tert*-butyl-functionalized Azobenzene (TBA) on Au(111). In this work we attempt a full *ab-initio* description of the explicit nuclear and electronic dynamics to analyze a novel substrate-mediated process that was suggested for this system [1]. The immense system size and a continuum of electronic states demand an effective modelling approach explicitly accounting only for the most important degrees of freedom. Employing an efficient density-functional theory based Δ SCF approach [2] we construct and analyze the involved excited-state potential energy surfaces (PESs), and establish a mixed-quantum classical dynamics simulation. A particular focus is the effect of the image-charge induced changes on the excited-state PESs and the excited-state lifetime- and temperature-dependence of the quantum yield. [1] Wolf, Tegeder, Surf. Sci. **603**, 1506–1517 (2009); [2] Maurer, Reuter, J. Chem. Phys. **139**, 014708 (2013)

CPP 34.12 Wed 18:00 ZEU 260

Reversible switching and light-induced structural changes in spin-coated thin films of Azobenzene-polymers — ●CHRISTOPHER WEBER¹, TOBIAS LIEBIG¹, DAVID BLÉGER², STEFAN HECHT², JÜRGEN RABE¹, and STEFAN KOWARIK¹ — ¹Humboldt-Universität zu Berlin, Institut für Physik — ²Humboldt-Universität zu Berlin, Institut für Chemie

Functionalized surfaces with molecules whose conformation can be reversibly switched between two isomeric forms by light are relevant for future devices -e.g. for switching adaptive materials, storing two states in memory applications, and switching current in molecular electronics. Here we use grazing incidence x-ray diffraction (GIXD), atomic force microscopy (AFM) and differential reflectance spectroscopy (DRS) to study light-induced structural changes in spin-coated thin films of Azobenzene-polymers with Alkyl side-chains. In solution, the individual Azobenzene-polymer shrinks upon UV-irradiation. Submonolayers of Azobenzene-polymers on Silicon oxide are still switchable with high efficiency, but do not show the same shrinking behavior, as suggested by AFM measurements before and after UV-illumination. Increasing the thickness to multilayers drastically changes the switching behavior, because of strong sterical hindrance. Interestingly, GIXD shows that the in-plane Bragg peaks corresponding to the coherent ordering of the Alkyl side-chains disappear when the sample is illuminated with UV-light and partially reappear after a few minutes in the dark, showing that switching is still possible in the crystalline state albeit with slower kinetics.

CPP 35: Biomaterials and Biopolymers (joint session with BP) I

Time: Wednesday 15:00–18:15

Location: ZEU 222

Invited Talk CPP 35.1 Wed 15:00 ZEU 222
Fabrication of 3D Cell Structures Using Self-Folding Polymer Films — ●LEONID IONOV — Leibniz Institute of Polymer Research Dresden

Nature offers an enormous arsenal of ideas for the design of novel materials with superior properties and interesting behaviors. In particular, self-assembly and self-organization, which are fundamental to structure formation in nature, attract significant interest as promising concepts for the design of intelligent materials. Self-folding stimuli-responsive polymer films are exemplary biomimetic materials and can be viewed as model systems for bioinspired actuation. Such films, on one hand, mimic movement mechanisms in certain plant organs and, on the other hand, are able to self-organize and form complex 3D structures. These self-folding films consist of two polymer layers with different properties. For such a bilayer to change its curvature at least one of these polymers, the active one, must change its volume more than the other one in response to changes in the external environment such as temperature, pH or light. Because of this non-equal expansion of polymers, these films are able to form tubes, capsules or more 3D complex structures. Self-folding polymeric films provide

unique possibilities for the straightforward fabrication of fibers with complex responsive architectures and that cannot be achieved using other currently available technologies. In this presentation, new applications of self-folding films for encapsulation and release of cells, 3D cell patterning as well as design of scaffolds will be demonstrated.

CPP 35.2 Wed 15:30 ZEU 222

Surface-Nanostructure Induced Structural and Dynamical Properties of Adsorbing Protein Layers — ●THOMAS F. KELLER¹, ROBERT SCHULZE², JÖRG BOSSERT², MARK KASTANTIN³, DANIEL K. SCHWARTZ³, and KLAUS D. JANDT³ — ¹Deutsches Elektronen Synchrotron (DESY), Hamburg, Germany — ²Friedrich Schiller University Jena, Germany — ³University of Colorado Boulder, USA

Designing implant surface properties on the nanoscale may be one method for tuning the structure and dynamics of adsorbing protein layers. For a set of materials with relevance in the biomedical field, such as ultra high molecular weight polyethylene (UHMWPE), titanium dioxide (TiO₂) and polystyrene-*b*-poly(ethylene oxide) (PS-*b*-PEO) block copolymers, we show how advanced materials processing permits the creation of surface nanostructures suitable for guiding ad-

sorbing proteins into lateral arrangements that may also affect their dynamic behavior, as determined from mapping using accumulated probe trajectories (MAPT). By atomic force microscopy (AFM), we observed that 1) the surface nanostructure of native UHMWPE may establish a densely packed, ordered arrangement of fibrinogen, which is one key protein in the implant-induced blood coagulation cascade, 2) adjacent crystalline facets on a nanostructured TiO₂ surface create local adsorption sites that guide fibrinogen into different conformational arrangements, and 3) nanoscale phase domains on block copolymer surfaces may serve as nucleation sites for fibrinogen networks. *Ref.: ACS Nano* **2011**, 5, 3120; *Adv. Funct. Mater.* **2012**, 22, 2617; *Acta Biomater.* **2013**, 9, 5810; *Macromolecules* **2012**, 45, 4740.

CPP 35.3 Wed 15:45 ZEU 222

On the Relationship between Peptide Adsorption Resistance and Surface Contact Angle: A Combined Experimental and Simulation Single-Molecule Study — •NADINE SCHWIERZ¹, DOMINIK HORINEK¹, SUSANNE LIESE², TOBIAS PIRZER¹, BIZAN N. BALZER¹, THORSTEN HUGEL¹, and ROLAND R. NETZ² — ¹Technische Universität München, Germany — ²Freie Universität Berlin, Germany

Controlling the adsorption of proteins and peptides at synthetic surfaces is the ultimate goal for designing biocompatible implants and fouling resistant surfaces. To gain a microscopic understanding of the transition between peptide adsorption and adsorption resistance, the force-induced desorption of single peptide chains is investigated in closely matched molecular dynamics simulations and atomic force microscopy experiments. In both simulations and experiments, the surfaces become adsorption resistant when their contact angle decreases below $\theta = 50^\circ$ - 60° , thus confirming the so-called Berg limit, established in the context of protein and cell adsorption.

Entropy/enthalpy decomposition of the simulation results reveals that the key discriminator between the adsorption of different residues on a hydrophobic monolayer is of entropic nature and thus is suggested to be linked to the hydrophobic effect. Peptide adsorption resistance is caused by the strongly bound water hydration layer and characterized by the simultaneous gain of both total entropy in the system and total number of hydrogen bonds between water, peptide, and surface. This mechanistic insight into peptide adsorption resistance might help to refine design principles for anti-fouling surfaces.

CPP 35.4 Wed 16:00 ZEU 222

Structural investigation of biomineralization processes in bio(mimetic)-materials by means of solid state NMR — •ANASTASIA VYALIKH and ULRICH SCHELER — Leibniz-Institut für Polymerforschung Dresden e.V.

Solid state NMR is applied to study the structure of biominerals. While the 31P solid state NMR spectra of phosphate containing materials represent a single broad line resulting from the diversity of structural motives, 2D heteronuclear correlation (HETCOR) experiments provide signal separation, and therefore can be used to determine the nature of mineral phases and interfacial organic-inorganic structures. The structure formation of biomimetic apatite-gelatine nanocomposites has been revealed, demonstrating the interaction of mineral domains with the organic matrix in the intergrowth region. HETCOR NMR provides resolution for the identification of different phosphate minerals at very early mineralization stages, which do not yet result in crystallite particles visible in imaging and diffraction techniques. The development of different calcium phosphate species in newly formed tissues has been demonstrated, when dental model implants were inserted in the mandible of minipigs and extracted after various healing time. While in mature bone hydroxyapatite, amorphous calcium phosphate and octacalcium phosphate are observed, the earlier stages include in addition β -tricalcium phosphate and brushite-like structures. We propose a method, which offers identification of biomineral components as well as the information on crystallite dimensionality based on strength of hydrogen bonds in water related structures.

CPP 35.5 Wed 16:15 ZEU 222

Elucidating insulin structure at hydrophobic interfaces — •SERGIO MAURI^{1,2}, TOBIAS WEIDNER², and HEIKE ARNLODS¹ — ¹Surface Science Research Centre, Department of Chemistry, University of Liverpool, UK — ²Max Planck Institute for Polymer Research, Mainz, Germany

Insulin unfolding and aggregation represents a hot topic for improving the delivery and storage of insulin based drugs.

Human insulin is a small peptide (51 amino acids) that regulates glycemia in the human body. It can be found in the form of hex-

amers, dimers and monomers: only the latter undergo unfolding and aggregation, forming fibril-like structures (amyloids).

It is generally known that interfaces trigger protein denaturation and eventually aggregation: in particular hydrophobic interfaces (such as the air/water interface) are known to disrupt insulin secondary structure, but the mechanism has not been explained in detail yet, since conventional spectroscopic methods do not have sufficient sensitivity to detect the interfacial protein layer.

Here we address this problem by applying a nonlinear optical technique, infrared-visible sum frequency generation, which is interface sensitive by virtue of optical selection rules and compare it to attenuated total internal reflection IR data at hydrophobic interfaces.

15 min. break

CPP 35.6 Wed 16:45 ZEU 222

A theoretical study of intermolecular interactions in crystalline cellulose — •JOHANNES HOJA and ALEXANDER F. SAX — Department of Chemistry, University of Graz, Graz, Austria

It is often claimed that cellulose I consists of sheets held together by van der Waals interactions and that each sheet consists of chains held together by hydrogen bonds. Since all weak intermolecular interactions consist of electrostatic, exchange, induction, and dispersion contributions we analyze in this study all intermolecular interactions in cellulose in terms of these four interaction contributions. It was shown that dispersion is crucial for the stabilization of alcohol dimers.[1] This justifies the use of a dispersionless density functional and an additional function that describes the dispersion contribution to the interaction energy for the investigation of the interactions in cellulose I α , I β , and II. For a better understanding of the nature of hydrogen bonds between cellulose chains we investigate model systems of alcohol dimers containing a different number of hydrogen bonds. Especially we study how the dimer stability depends on the intermonomer distance and the topology of the hydrogen bonding networks. For these investigations we use symmetry-adapted perturbation theory based on DFT description of monomers [SAPT(DFT)]. We find that dispersion is not only responsible for the intersheet stabilization but also contributes significantly to the intrasheet interactions. This is in opposition to the general view that only electrostatic interactions are important for hydrogen bonding.

[1] Hoja et al., Chem. Eur. J., DOI: 10.1002/chem.201303528, in press.

CPP 35.7 Wed 17:00 ZEU 222

Biomodified, stimuli responsive surface coatings based on polymer brushes — •EVMORFIA PSARRA^{1,2}, ULLA KÖNIG¹, KLAUS-JOCHEN EICHHORN¹, MANFRED STAMM^{1,2}, and PETRA UHLMANN¹ — ¹Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany — ²Technische Universität Dresden, Physical Chemistry of Polymer Materials, Dresden, Germany

The main focus of this work is the surface biofunctionalization of ultrathin, stimuli responsive polymer brushes grafted to model surfaces. Different polymer brushes either composed out of a pH responsive component, the Poly(acrylic) acid (PAA), and/or a temperature responsive material, the Poly(N-isopropyl acrylamide) (PNIPAAm) are used to investigate the Arg-Gly-Asp (RGD) peptide binding to the brush surface. Using PNIPAAm mixed with PAA polymer material in order to generate binary brushes will help to create smart surface coatings which are hiding or exposing their functionalities by changing the temperature from physiological (37°C) to room temperature. Binary brushes functionalized with cell-signaling molecules, can lead to intelligent stimuli-responsive bio-nanosurfaces, able to regulate cell adhesion and function. Here we are presenting detailed surface analysis results for the PNIPAA-PAA RGD modified system.

CPP 35.8 Wed 17:15 ZEU 222

Microtopographic substrates for controlling cell adhesion at the nanoscale — •LAITH KADEM, JULIA PURTOV, CONSTANZE LAMPRECHT, and CHRISTINE SELHUBER-UNKEL — Biocompatible Nanomaterials, Institute for Materials Science, University of Kiel

Diblock-copolymer micelle nanolithography has in recent years proven to be a valuable tool for controlling the adhesion of cells at the nanoscale by offering a control over spacing variation in binding sites of single-cell adhesion receptors. Here we present a novel method to additionally control binding sites spacing on regular micropatterns. We use a micro-structured topography on Si substrates that can be

easily produced with photolithography followed by wet etching. Performing a diblock-copolymer micelle nanolithography procedure on such substrates introduces nanoparticle arrays of different densities and spacings in the pattern provided by the microtopography in a single-step. With this technique, we can achieve spacing variations in the micropattern of up to 25 nm. The microstructured domains patterned with nanoparticle arrays were biofunctionalized with RGD ligands in order to make them attractive for integrin binding in order to further study the effect of ligand spacing on cell adhesion. Thus, our micro-patterned nanostructured surfaces now provide a versatile platform for studying cellular adhesion processes that are influenced by micro-nanostructured ligand spacing and density.

CPP 35.9 Wed 17:30 ZEU 222

Thermal Melting of Protein Beta Sheet Crystals — ANDREAS WURM¹, EVGENY ZHURAVLEV¹, XIAO HU², DAVID KAPLAN², PEGGY CEBE², and CHRISTOPH SCHICK¹ — ¹University of Rostock, Institute of Physics, Germany — ²Tufts University, Medford MA, USA

The remarkable stability that makes silk useful in garments and surgical sutures has impeded efforts by scientists to study its thermo-physical properties. Here, we use fast scanning chip calorimetry and report the first reversible thermal melting of protein beta-pleated-sheet crystals, exemplified by silk fibroin. Heating nanogram-sized samples at 2000K/s, allowed us to avoid thermal decomposition, and demonstrate that beta-pleated-sheet crystals melt to become random coils, helices and turns. We establish that following melting silk can be recrystallized into beta-pleated-sheets, and remelted. The similarity between thermal melting behavior of beta-pleated-sheet crystals and crystals of synthetic polymers is confirmed. Significance for controlling beta-pleated-sheet content during thermal processing of biomaterials is

envisioned based on these findings. Demonstration of reversible thermal transitions in silk, the most beta-pleated-sheet-enriched and stable protein, suggests important new insights can also be gained with the broader range of proteins where beta-pleated-sheets serve as critical control points in structural transitions.

Invited Talk CPP 35.10 Wed 17:45 ZEU 222
Biopolymer Network Mechanics: Nonlinearity and Hierarchy. — ●CORNELIS STORM — Department of Applied Physics and Institute for Complex Molecular Systems, Eindhoven University of Technology, The Netherlands.

Biological materials possess some remarkable mechanical properties. Cells and tissues can adjust, remodel, stiffen, soften, in some cases even pack up and leave when circumstances require action. Surprisingly, most systems that exhibit this stunningly complex response, such as the cytoskeleton inside cells and the extracellular matrix, share a common design: under a microscope, they are crosslinked, hierarchical networks of biological polymers. Even more surprisingly, many of the in vivo behaviors can be reproduced in vitro in reconstituted proteinaceous polymer gels. Many of these systems, most notably collagen, play a purely structural role in living organisms. In other words, their function is their mechanical response. Biopolymer networks are therefore particularly suited to begin to understand the complex relationship between structural design and functionality in living systems.

In this seminar, I will discuss our efforts to bridge the gap from microscopic structure to macroscopic mechanical response of such nonlinear systems using collagen as an example. Towards the end, I will discuss our first steps towards controlling the nonlinear mechanical properties of biomimetic synthetics.

CPP 36: Colloids and Complex Liquids II

Stabilization, Flow/Fields

Time: Wednesday 15:00–18:15

Location: ZEU 114

CPP 36.1 Wed 15:00 ZEU 114

Colloidal stabilization by unattached homopolymers, when does depletion repulsion play a role — ●JOCHEN SCHNEIDER and ECKHARD BARTSCH — Institut für Makromolekulare Chemie/Institut für Physikalische Chemie – Albert Ludwigs Universität Freiburg, Deutschland

It is well known that the addition of non-adsorbing polymers to a dispersion of hard sphere like (HS) colloidal particles introduces short range attraction to the system. This so called depletion attraction can be used to study flocculation or the phase-behaviour of colloidal systems with short range attraction. Beside this polymer-induced (PI) attraction in some cases a PI repulsion can be observed. So far a (re-)stabilisation of a flocced phase by PI repulsion could only be observed in sterically stabilised particles having thick stabilisation layers. Whether restabilisation can be realised in a true HS system is not yet known. Recently Semenov et al. published theoretical work on colloid-polymer-mixtures, where they predicted restabilisation in a HS system in the case of large particles and much smaller polymers, but these predictions have not yet been tested experimentally.

To gain experimental access to the influence of PI interactions on particle interactions, we study the osmotic compressibility of HS systems using turbidimetry. So far similar experiments were only carried out on rather small particles, where PI repulsion is of no importance. Thus we are extending the method towards larger particle sizes to check whether the PI stabilisation described by Semenov is able to give a more satisfying description of the data than the classic approaches.

CPP 36.2 Wed 15:15 ZEU 114

The collapse of colloidal monolayers by capillary attraction — JOHANNES BLEIBEL¹, ALVARO DOMINGUEZ², and ●MARTIN OETTEL¹ — ¹Institut für Angewandte Physik, Universität Tübingen — ²Fisica Teorica, Universidad de Sevilla

We investigate the evolution of a system of colloidal particles trapped at a fluid interface and interacting via capillary attraction, as function of the range of the capillary interaction and temperature. We address the collapse of a homogeneous particle distribution and of a radially symmetric (disk-shaped) distribution of finite size, both theoretically

by using a perturbative approach inspired by cosmological models, as well as numerically by means of Brownian Dynamics and Dynamical Density Functional Theory. We find a “dynamic phase diagram”, exhibiting a smooth crossover from collective (gravitational-like) collapse to local (spinodal-like) clustering. In the crossover region, the evolution exhibits a peculiar shock wave behavior at the outer rim of the disk-shaped distribution.

CPP 36.3 Wed 15:30 ZEU 114

Fluorescence Correlation Spectroscopy Directly Monitors the Equilibrium Chain Exchange Kinetics of Diblock Copolymer Micelles — ●DAVID SCHAEFFEL, ANDREAS KREYES, YI ZHAOU, DANIEL CRESPIY, KATHARINA LANDFESTER, HANS-JÜRGEN BUTT, and KALOIAN KOYNOV — Max Planck Institute for Polymer Research, Mainz, Germany

We present a new method for monitoring the equilibrium exchange kinetics of building molecules between amphiphilic diblock copolymer micelles. The method is based on dual color fluorescence cross correlation spectroscopy (DC FCCS) and offers single molecule sensitivity. We demonstrate its versatility by studying polystyrene-block-poly[oligo(ethylene glycol) methyl ether methacrylate] (PS-b-POEGMA) micelles in different selective solvents and solvent-mixtures at various temperatures. If pure water is used as a selective solvent, no exchange could be observed at temperatures below the glass transition of the core forming PS block. In methanol, the exchange persists even at temperatures well below the PS glass transition suggesting that the methanol swells the micelles core. However, adding only small amounts of bad or good solvents can slow down or fasten the kinetics by orders of magnitude. Our findings demonstrate that DC FCCS is a fast and reliable tool to study the dynamic equilibrium exchange kinetics of copolymer micelles.

CPP 36.4 Wed 15:45 ZEU 114

Sub-millisecond dynamics of vesicles formation — ●RITA GRACEFFA^{1,2}, SAGAR V. KATHURIA³, RAUL A. BARREA¹, R. PAUL NOBREGA³, SRINIVAS CHAKRAVARTHY¹, OSMAN BILSEL³, THOMAS C. IRVING¹ und THOMAS M. WEISS⁴ — ¹BioCAT, CSRR and Department BCS, Illinois Institute of Technology, 3101 South Dearborn, Chi-

cago, IL 60616, USA — ²Institute for X-ray Physics, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — ³Department of Biochemistry and Molecular Pharmacology, University of Massachusetts Medical School, 364 Plantation Street, LRB 919, Worcester, MA 01605, USA — ⁴Stanford University, Stanford Synchrotron Radiation Lightsource, 2575 Sand Hill Rd. MS69, Menlo Park, CA 94025, USA

Recently, the formation of vesicles has been studied in situ at millisecond time-scales and disk like intermediate states have been shown to exist in some mixed systems composed of zwitterionic and anionic surfactants. However, for vesicle formation from cationic-anionic surfactant mixture no such intermediates could be detected at the achieved time resolution.

We present a study of dynamics formation of unilamellar vesicles from a mixture of oppositely charged surfactants in the microseconds range. The vesicles spontaneous self-assembly was investigated by mixing anionic and cationic micelles in a micro-mixer. The reaction intermediates were probed with Small Angle X-ray and Förster Resonance Energy Transfer. The formation of the vesicles happens within the mixing time, 100 microseconds.

CPP 36.5 Wed 16:00 ZEU 114

Effects of flow on topological defects in a nematic liquid crystal near a colloid — ●TILLMANN STIEGER¹, MARTIN SCHOEN^{1,2}, and MARCO G. MAZZA³ — ¹Technische Universität Berlin, Straße des 17. Juni 115, 10623 Berlin, Germany — ²North Carolina State University, 911 Partners Way, Raleigh, North Carolina 27695, USA — ³Max Planck Institut für Dynamik und Selbstorganisation, Am Faßberg 17, 37077 Göttingen, Germany

Microfluidic applications are becoming an extremely important tool to manipulate fluids, droplets and materials at small scales. Anisotropic liquids are a promising novel approach to such applications. However, a clear understanding of the modifications induced by flow when a colloid is immersed in a liquid crystal is still missing. Our molecular dynamics simulations show that flow has in fact a significant impact on defect structures around a colloidal particle. We show that flow distorts Boojum defects into an asymmetrically larger downstream lobe, and that Saturn ring defects are convected downstream along the flow direction, which is in agreement with experimental observations [1]. Additionally, for a Janus colloid with both parallel and perpendicular patches, exhibiting a Boojum defect and a Saturn ring defect, we find that the Boojum defect facing the upstream direction is destroyed and the Saturn ring is convected downstream.

[1] S. Khullar, C. Zhou, and J. J. Feng, *Phys. Rev. Lett.* **99**, 237802 (2007).

CPP 36.6 Wed 16:15 ZEU 114

New fitting model for structural oscillation forces — ●SEBASTIAN SCHÖN — Technische Universität Berlin Strasse des 17. Juni 124 D-10623 Berlin

Structural forces are a well known phenomenon in surface science. They arise due to the layering of particles in the vicinity of a confining wall. The layered structure has an oscillatory density profile in normal direction. Overlap with a second interfacial region results in an attractive or repulsive force acting on the surfaces, depending on the separation of the walls. These forces can be fitted via following formula:

$$f(x) = -A \cdot e^{-x/\xi} \cdot \cos(2\pi(x - \Delta x)/\lambda),$$

where f is the force, x is the separation between the walls, A is the amplitude of the oscillations, ξ is the decay length, λ signifies the wavelength of the oscillation and Δx is the phase shift. This common fit formula can be extended by introducing an additional term of exponential decaying nature. The additional term is able to describe deviations between the common fit and data measured for aqueous suspensions of silica nanoparticles, especially at small wall to wall separations and larger concentrations. Furthermore, it is shown that neglecting this term leads to an oscillatory behaviour depending on the starting point of the fit region of the three important fit parameters: amplitude, wavelength and decay-length. The extension enables a large increase of the data range accessible for accurate fitting, especially towards small separation and leads to the removal of the oscillatory behaviour of the fit parameters. Therefore, resulting in a strong increase of accuracy for all fit parameter in the system studied here.

15 min. break

CPP 36.7 Wed 16:45 ZEU 114

Shear banding in weakly attractive soft jammed materials — ●EHSAN IRANI¹, PINAKI CHAUDHURI², and CLAUS HEUSSINGER¹ — ¹Institut für Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany — ²Heinrich Heine University of Düsseldorf, Düsseldorf, Germany

We study the rheology of a system of weakly attractive soft particles close to jamming. Lees-Edward boundary conditions are used to impose a shear flow in two dimensions. Shear stress as a function of shear rate shows non-monotonic behavior signaling a mechanical instability. This leads to persistent spatial heterogeneities in flow, which becomes prominent with increasing system size. In the yield stress regime, a fragile solid is formed even far below the jamming point. A scaling argument is presented that connects the yield stress to the attraction strength and the connectivity of the fragile solid. The shear-banding instability is explained with the breakdown of the solid and an associated loss of structure. This mechanism could be a scenario to explain shear banding in different materials with short-range attractive forces.

CPP 36.8 Wed 17:00 ZEU 114

Writing nanoparticles lines: in-situ observation of structure formation — ●BERIT HEIDMANN¹, MATTHIAS SCHWARTZKOPF¹, ROMAN MANNWEILER¹, STEPHAN V. ROTH¹, FRANS DE JONG², and MICHAEL SCHLÜTER² — ¹DESY, Notkestr. 85, 22607 Hamburg — ²Institute of Multiphase Flows, TUHH, Eißendorfer Str. 38, 21073 Hamburg

Adsorption of colloids on surfaces allows for tailored installation of ordered arrays of nano- and mesostructures [1]. Here, it is crucial to understand the adsorption process in-situ and follow the deposition and ordering of the colloids in line-type structures. For our in-situ investigation, we use a combination of microbeam grazing incidence small-angle x-ray scattering (GISAXS) and contact angle apparatus. The high-precision dosing system enables us to write line-type structures over macroscopic distances by depositing colloids from an aqueous solution (sub microliter) volume of nanoparticles. Such structures are useful for establishing complex conducting pathways on organic substrates without the use of designed masks. GISAXS enables us to detect the various stages of nanostructure formation, identifiable by the characteristic scattering of the gold colloids being adsorbed and chemically bound to the functionalized silicon. We present our results on the specific system gold nanoparticles on Mercapto-Propyl-Trimethoxysilanized silicon surface and correlate our nanostructural finding with UV-Vis measurements. [1] Wu, T.-H., Lu, H.-H. and Lin, C.-W., Dependence of Transport Rate on Area of Lithography and Pretreatment of Tip in Dip-Pen Nanolithography, *Langmuir*, 2012, 28, 14509-14513

CPP 36.9 Wed 17:15 ZEU 114

Stress-driven Dynamic Behavior of Free-Standing Bent-Core Liquid Crystal Filaments — ●TANYA OSTAPENKO¹, SEYYED MUHAMMAD SALILI², ALEXEY EREMIN¹, ANTAL JÁKLI², and RALF STANNARIUS¹ — ¹Institute of Experimental Physics, Otto-von-Guericke-Universität, 39106 Magdeburg, Germany — ²Chemical Physics Interdisciplinary Program and Liquid Crystal Institute, Kent State University, Kent, OH 44242, USA

Filament forming materials, such spider silk, collagen and cellulose, are widespread in nature [1]. The B₇ liquid crystalline phase of bent-core mesogens is an exceptionally good example of a mesophase forming very stable fluid filaments [2]. This phase is distinguished by an internal structure of strongly undulated molecular layers and spontaneous polarization with local splay. This results in an overall chiral columnar structure.

Here, we report on the dynamic behavior of free-standing bent-core liquid crystal filaments under dilative and axial compressive stresses in the B₇ phase [3]. We found that such filaments demonstrate very complex structures depending on the filament's temperature relative to the clearing point, initial filament thickness, and on the velocity at which the filament is pulled or compressed. We discuss possible reasons for the formation of such structures.

[1] F. Vollrath, D. Knight. *Nature* **410**, 541 (2001).

[2] A. Jákli, D. Krüerke, and G.G. Nair, *Phys. Rev. E* **67** (2003).

[3] T. Ostapenko, S.M. Salili, A. Eremin, A. Jákli, and R. Stannarius (submitted).

CPP 36.10 Wed 17:30 ZEU 114

Gradient diffusion in ferrofluids with chain aggregates — ●ALLA MURATOVA¹, ALEXEY IVANOV¹, and SOFIA KANTOROVICH^{1,2} — ¹Ural Federal University, 620000, Russia, Ekaterinburg, Lenin. av., 51

— ²University of Vienna, Sensengasse 8, 1090, Wien, Austria

We present the results on the mobility and diffusion coefficients in the systems of magnetic dipolar particles. There were several attempts to study diffusion [Yu. A. Buyevich et al., *Physica. A* 190, 276 (1992); P. Ilg, *Phys. Rev. E* 71, 051407 (2005); J. Jordanovic et al., *Phys. Rev. Lett.* 106, 038301 (2011)], but the detailed theoretical description is still missing. We study how the mobility and diffusion coefficients depend on the system polydispersity, granulometric composition, geometrical constraints, and a presence of an external magnetic field. In order to know this, we consider three-dimensional and quasi-two-dimensional mono- and bidisperse systems with and without an external magnetic field. We use the obtained diffusion coefficients for calculating the distribution of chain aggregates in the gravity gradient. Also we consider different systems in dependence of different particle sizes. The main method of our theory is density functional theory. We compare our theoretical results, and explain dependence of the diffusion coefficients on some parameters. Also we compare our theoretical results to the data of the computer simulations.

CPP 36.11 Wed 17:45 ZEU 114

Smoothed particle hydrodynamics of complex fluids — •DANIEL RINGS and PETER OLMSTED — University of Leeds

The rheology of complex liquids such as polymer solutions is of great interest in various disciplines and the commonly used theoretical research tools range from analytic phenomenological models to large-scale molecular dynamics simulations. Smoothed particle hydrodynamics (SPH) is a promising hybrid method which combines microscopic detail of a certain extent with computational efficiency. Originally invented for astrophysical calculations, this Lagrangian method approximates the solution to the (slightly compressible) Navier–Stokes equations by smoothly interpolating the fields which are evaluated at advected virtual particles. The appeal of this method is its relative ease to deal with complicated boundary conditions without the need

for mesh construction and to capture spatial inhomogeneities and temporal transients. Last but not least, it can be implemented on the basis of existing molecular dynamics software.

For a fluid with a non-monotonic flow curve, we study in detail the shear banding transition and how it is affected by the presence of immersed rigid colloids. We discuss discrepancies between different apparent stress states and comment on the interpretation of results obtained within the framework of SPH—of particular interest in view of the growing use of this method in computational fluid dynamics.

CPP 36.12 Wed 18:00 ZEU 114

Melting liquid and crystalline droplets in rod-sphere dispersions by shear flow — •DONALD GUU¹, MINNE PAVLIK LETTINGA^{1,2}, and JAN KAREL GEORGE DHONT^{1,3} — ¹Forschungszentrum Juelich, Institute of Complex Systems 3, Leo-Brandt-Str, 52425 Juelich, Germany — ²Department of Physics and Astronomy, Laboratory for Acoustics and Thermal Physics, KU Leuven, Celestijnenlaan 200D, Leuven B-3001, Belgium — ³Heinrich-Heine-Universitaet Duesseldorf, Universitaetsstrasse 1, 40225 Duesseldorf, Germany

We determined the phase behavior of an ideal rod*sphere mixture consisting of fd-virus, which are mono-disperse colloidal rods, and density matched mono-disperse polystyrene spheres, using a combination of diffuse wave spectroscopy and optical microscopy. Equilibrium phase diagrams were mapped out for various L/R ratios, where L is length of the rod and R is the sphere radius. At high L/R we observe droplets of a liquid phase of the spherical particles, while at lower L/R we obtained clusters which are crystalline. We studied the susceptibility of the droplets to shear flow, using a counter rotating cone-plate shear cell mounted on a fast confocal microscope. We observed a shear rate dependent melting of the structures, which is a function of the location in the equilibrium phase diagram of the sheared mixture. We show that the melting of liquid droplets takes place via another mechanism than for the crystalline clusters.

CPP 37: Poster Session 2

Polymer Dynamics, Rheology, Polymer Globules, Wetting, Micro- and Nanofluidics, Interfaces and Thin Films, Crystallization, Nucleation and Self Assembly

Time: Wednesday 15:00–19:00

Location: P3

CPP 37.1 Wed 15:00 P3

Interactions between Water and Linear Poly(N-isopropylacrylamide) Chains Around the Phase Transition Investigated by Dielectric Relaxation Spectroscopy — •MARIEKE FÜLLBRANDT^{1,2}, ELENA ERMILOVA³, ASAD ASADUJAMAN¹, RALPH HÖLZEL³, FRANK F. BIER³, REGINE VON KLITZING², and ANDREAS SCHÖNHALS¹ — ¹BAM Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12205 Berlin — ²Technische Universität Berlin, Strasse des 17. Juni 124, 10623 Berlin — ³Fraunhofer-Institut für Biomedizinische Technik IBMT, Am Mühlenberg 13, 14476 Potsdam

The molecular dynamics of linear poly(N-isopropylacrylamide) (pNIPAM) in aqueous media are investigated using dielectric relaxation spectroscopy in a frequency range from 0.1 Hz to 100 GHz. Below the lower critical solution temperature (LCST) two relaxation processes are observed located in the MHz and GHz region assigned to the reorientation of dipoles of the solvated polymer segments (p-process) and water molecules (w-process), respectively. Both relaxation processes are analyzed using the Havriliak-Negami (HN) functions taking special attention to the w-process. Above the LCST the dielectric spectra of the pNIPAM solutions resemble that of pure water showing only the high frequency relaxation process of the water molecules with more or less Debye-type behaviour. The non-Debye behaviour of the w-process below the LCST is mainly induced by the interactions between water and pNIPAM chains via hydrogen bonding. The relaxation time and strength of the w-process is studied in dependence on the concentration, temperature and the polymer chain length.

CPP 37.2 Wed 15:00 P3

Different Polymer Architectures under External Oscillatory Forces — •RON DOCKHORN^{1,2}, TOM GIESSGEN^{1,2}, and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden e.V., D-01069 Dresden, Germany — ²Technische Universität Dresden, In-

stitut für Theoretische Physik, D-01069 Dresden, Germany

We are studying the force-extension behavior of different polymer architectures (linear chains, ring polymer, ₃₁-trefoil knot, two connected or concatenate rings) by using the bond-fluctuation simulation method. First, we apply a constant force f_0 on the chain ends and determine the response of the end-to-end-distance R . The simulation results for the linear and ring structures follow the scaling prediction of the linear $\sim f_0$ and Pincus-regime $\sim f_0^{2/3}$, but the connected/concatenate rings show small deviations. Second, we apply an oscillatory force $f = f_0 + f_a \cdot \sin(\omega t)$ acting on the chain ends and investigate the response of the end-to-end-distance R on the oscillatory frequency ω . An analytical expression for the end-to-end-distance $R(f)$ is derived by using the Rouse model. For the dissipation of energy we are calculating the hysteresis loop $A = \oint dfR(f)$ and find a maximum of hysteresis if $\omega\tau_R = 1$ for ideal structures with τ_R as Rouse time which is confirmed by the simulations. The hysteresis for the different polymer architectures follow the predicted trend, but show specific deviations.

CPP 37.3 Wed 15:00 P3

Molecular dynamics of poly(cis-1,4-isoprene) in 1- and 2-D confinement — •EMMANUEL URANDU MAPESA¹, MARTIN TRESS¹, WYCLIFFE KIPROP KIPNUSU¹, MANFRED REICHE², and FRIEDRICH KREMER¹ — ¹Institute for Experimental Physics I, University of Leipzig, Leipzig, Germany — ²Max-Planck Institute for Microstructure Physics, Weinberg, Halle (Saale), Germany

Broadband Dielectric Spectroscopy - in combination with a nanostructured electrode arrangement - is employed to study thin layers of poly(cis-1,4-isoprene) (PI). PI is further probed in the 2-D confining space of Anodic Aluminium Oxide (AAO) nanopores. We report that while the structural relaxation shows dependence on neither layer thickness nor molecular weight, the normal mode is dramatically influenced by confinement: (i) its relaxation strength is layer-thickness-dependent; (ii) for PI having a molecular weight Mw comparable to

M^* (i.e. the critical molecular weight below which Rouse dynamics dominate), the mean spectral position does not shift with layer thickness, (iii) in contrast, when $M_w > M^*$, the relaxation strength and rate of the normal mode respond to the confinement; (iv) it is demonstrated, for the first time, that the polymer solution from which the thin layers are spincoated has an impact on the chain dynamics; and (v) the extent by which the normal mode is affected depends on the dimensionality of confinement. Put together, these results show that while the chain dynamics are altered in a manifold of ways (due, for instance, to interactions with the confining surface), the dynamic glass transition retains most of its bulk-like nature.

CPP 37.4 Wed 15:00 P3

Photorefractive Effect in Azobenzene-Containing Materials — ●CHRISTOPH MEICHNER¹, LOTHAR KADOR¹, CHRISTIAN PROBST², ROBIN PETTAU², 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

Azobenzene-based materials are usually used for holographic applications. Recent measurements reveal that they also exhibit a photorefractive effect. It manifests itself in intensity variations of the two transmitted laser beams (488 nm) which are used for hologram inscription (so-called asymmetric two-beam coupling). This effect has its origin in a phase shift between the holographic light intensity grating and the refractive-index grating in the material. The difference to most two-beam coupling experiments in other materials is that the effect arises here without any external electrical field applied. The measurements show that the phase difference is dynamical and varies with time.

CPP 37.5 Wed 15:00 P3

Spatially Resolved Single Molecule Spectroscopy in Thin Semi-Crystalline Polypropylene Films — ●GORDON HERWIG, STEFAN KRAUSE, MARTIN NEUMANN, ROBERT MAGERLE, and CHRISTIAN VON BORCZYKOWSKI — Technische Universität Chemnitz, Fakultät für Naturwissenschaften, Chemnitz, Germany

The fluorescence of a single molecule is a sensitive indicator for its environment. Changes of the fluorescence lifetime, emission wavelength and polarization can report spatial and temporal changes within the vicinity of the dye. Here we report on confocal microscopy studies of single perylene diimides in thin films of semi-crystalline polypropylene with a spatially complex microstructure on the nanometer scale. The velocity of the orientational diffusion is measured and correlated with the information about the dye's local environment. The latter is obtained from high-resolution atomic force microscopy (AFM) images of the specimen's microstructure. Fluorescent particles that are visible in both confocal microscopy and AFM images are used for image registration with high spatial accuracy. This allows us to determine the position of individual dye molecules between crystalline lamellae and provides insight into the dye's local mobility, which is related to the local viscosity within the amorphous regions of polypropylene.

CPP 37.6 Wed 15:00 P3

Single Molecule Reorientation Dynamics in Deformed Polymethylacrylate Melts — ●STEFAN KRAUSE, MARTIN NEUMANN, ROBERT MAGERLE und CHRISTIAN VON BORCZYKOWSKI — Fakultät für Naturwissenschaften, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

The fluorescence of a single molecule (SM) is a very sensitive probe for the molecules environment and changes of the fluorescence lifetime, emission wavelength, and polarization can report spatial and temporal changes in the environment of the fluorescent dye. Here we report on polarization sensitive SM microscopy in thin films of polymethylacrylate (PMA) melts that are stretched in a microtensile testing setup. Functionalized perylene diimide dyes embedded in the PMA film report their molecular reorientation dynamics and changes within their local environment via polarization sensitive SM microscopy. In control experiments we studied the stress-strain behaviour and the stress relaxation of the PMA films. This experiment provides insights into the steric coupling processes between fluorescent probe molecules and polymer chains which are not accessible with other microscopy techniques. The data show a continuous transition from an anisotropic distribution of orientations to a more isotropic distribution during deformation of the polymer. In addition, the experiment allows for the direct observation of reorientation of the molecules after deformation

which is in close relation with the relaxation of the polymer films.

CPP 37.7 Wed 15:00 P3

Structure and Dynamics of High-temperature Polymer Electrolyte Fuel Cells investigated by Neutron Scattering — ●BERNHARD HOPFENMÜLLER¹, OXANA IVANOVA¹, OLAF HOLDERER¹, WIEBKE MAIER², WERNER LEHNERT², REINER ZORN³, and MICHAEL MONKENBUSCH³ — ¹JCNS, Forschungszentrum Jülich GmbH, Outstation at MLZ, Garching, Germany — ²IEK-3, Forschungszentrum Jülich GmbH, Jülich, Germany — ³JCNS-1 & ICS, Forschungszentrum Jülich GmbH, Germany

High-temperature polymer electrolyte fuel cells based on (poly(2,2'-(m-phenylene)-5,5'-bibenzimidazole) membranes (PBI) with phosphoric acid impregnation are a new promising material for high-temperature polymer electrolyte fuel cells (HT-PEFCs). Their operating temperatures are above the boiling point of water. PBI membranes show good chemical resistance and high glass transition temperature (about 700 K). After being loaded with phosphoric acid (PA) such membranes provide very good proton conductivity ($\sim 80\text{mS/cm}$ at 140°C), which increases with an increasing amount of PA in the system [1,2] Different neutron scattering techniques, including back scattering, small-angle-neutron-scattering or time-of-flight-scattering are practical to investigate structure and dynamics in these systems. We will present results obtained from such measurements.

[1] C. Wannek, W. Lehnert, J. Mergel, J. Power Sources 192 (2009) 258. [2] Q. F. Li, J. O. Jensen, R. F. Savinell, N. J. Bjerrum, Progress in Polymer Science 34 (2009) 449.

CPP 37.8 Wed 15:00 P3

ReaxFF reactive force field model for Twin Polymerization — ●THOMAS SCHÖNFELDER¹, JOACHIM FRIEDRICH², STEFFEN SEEGER¹, JANETT PREHL¹, and KARL HEINZ HOFFMANN¹ — ¹Department of Physics, Computational Physics, TU Chemnitz — ²Department of Chemistry, Theoretical Chemistry, TU Chemnitz

Twin polymerization is a new synthesis concept which enables the formation of two different macromolecular structures from organic-inorganic hybrid materials in one single process step [1]. It is characterized by two main process types - electrophilic substitutions contributing to the organic network formation and condensation reactions building the inorganic structure for the reviewed monomer 2,2*-spirobi[4H-1,3,2-benzodioxasiline]. To understand the formation process we develop a first-principles-based ReaxFF reactive force field for C/O/H/Si(S,F,Ti,...).

The corresponding parameterizations known in literature are not able to describe the twin polymerization process to its full extent.

Here, we present our adapted ReaxFF model, so that the first steps of the twin polymerization are captured properly.

[1] Nanocomposites Prepared by Twin Polymerization of a Single-Source Monomer. S. Grund, P. Kempe, G. Baumann, A. Seifert, S. Spange, Angew. Chem. Int. Ed. 2007, 46, 628-632. DOI: 10.1002/anie.200504327

CPP 37.9 Wed 15:00 P3

Relaxation Processes Interpreted as Low-Pass Filters — ●LOTHAR KADOR — University of Bayreuth, Institute of Physics and BIMF, 95440 Bayreuth

Many systems in physics perform relaxation processes upon external stimulation. Examples are glasses investigated with dielectric spectroscopy and fluorescing or phosphorescing chromophore molecules after absorbing appropriate optical frequencies. When the stimulation is modulated, relaxing systems behave like electronic low-pass filters: Low modulation frequencies are transmitted without attenuation, signals of high frequencies are integrated and experience a phase shift. If the relaxation is single-exponentially, there is full equivalence to a simple RC low pass; more complicated relaxation laws correspond to low-pass filters of higher order. Measurements of the relaxation behavior in the frequency domain and the corresponding filtering behavior are interpreted in terms of the Cole-Cole or polar plot. Special situations arise, when the system responds non-linearly to the external stimulation.

CPP 37.10 Wed 15:00 P3

NMR-Investigations of Semicrystalline Polymers — ●RICARDO KÜRZ — Martin-Luther Universität Halle-Wittenberg, Institut für Physik, Betty Heimann Straße 7, 06120 Halle (Saale)

The dynamics of semicrystalline polymers Poly-Capro-Lactone and

Poly-Ethylene-Glycole have been investigated by the approach of solid-state NMR.

CPP 37.11 Wed 15:00 P3

Specific Interactions In A Coarse Grained Hard Sphere 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 use an off-lattice hard-sphere coarse grained model with a square well (sw) potential for studying structure formation of homopolymer chains. Starting with tangent spheres, shortening of the bond length introduces stiffness. Due to this bond length reduction the spatial structure changed from crystalline to helical-like structures within the lower energy range of the density of states (DOS). We introduce a further interaction where predefined pairs interact via an additional sw potential. This allows the chain to reach lower energy states and leads to a stabilization of additional structures which will be shown in the analysis of thermodynamic functions. For an improved performance for estimating the DOS, the Stochastic Approximation Monte Carlo method is paired with a consecutive Umbrella Sampling.

CPP 37.12 Wed 15:00 P3

In situ x-ray studies of P3HT based bulk heterojunction (BHJ) solidification — ●CHRISTELLE KWAMEN¹, EDUARD MIKAYELIAN¹, PANAGIOTHIS KARAGIANNIDIS², STERGIOS LOGOTHETIDIS², and SOUREN GRIGORIAN¹ — ¹Soft Matter Physics Group, University of Siegen, Siegen Germany — ²LTNF, Physics Department, Aristotle University of Thessaloniki, Thessaloniki Greece

Over the years, the performance of bulk heterojunction(BHJ) polymer solar cells has been shown to be dependent of the local morphology of the active layer. Many processing techniques have been explored to improve the structure of the BHJ layer, passing through solvent, concentration, mixture ratio, thermal annealing etc.(1)

Grazing incidence X-ray diffraction measurements performed on annealed and pristine P3HT:PCBM films showed a strong enhancement of P3HT structure making the (020) peak of π - π stacking visible after annealing. For in situ research, we monitored the solidification of BHJ films where the current- voltage characteristics were recorded simultaneously with GIXD patterns in real time during film formation(2). The structural properties of P3HT-based BHJ and their correlation to electrical performance will be discussed.

This work was partly supported by BMBF (project Nr 05K13PS4).

References: (1)*Al.Ibrahim, M. et al., Appl.Phys.Lett.86 201120(2005) (2)*Grodd L. et al., Macrom. Rapid Comm. 2012, 33(20),1765-1769

CPP 37.13 Wed 15:00 P3

Surface modification, colloidal interaction and the motion of particles — JENNIFER WENZL¹, RYOHEI SETO^{1,2}, and ●GÜNTER K. AUERNHAMMER¹ — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²Benjamin Levich Institute for Physico-Chemical Hydrodynamics, New York, NY 10031, United States

A large portion of the goods transported on earth is transported as granulates and powders. With the advances in production techniques of composite materials, the grain size of these powders tends to shrink and reach sizes in the micron and even sub-micron range. For a good processability of the powders their flow behavior is a dominant parameter. The smaller the particles become, the more dominant is the influence of the inter-particle forces on this flow behavior. The macroscopic behavior of such particulate systems is a complex interplay between the internal properties of the particles, their surface properties and the structure the particles form. In this presentation I will focus on the effect of the particle surface and its modification.

I will discuss the influence of surface modification and particle interaction on the mobility of the particles on various length scales. By choosing the appropriate particle chemistry, the interaction between the particles can be tuned from attractive and strongly binding to almost purely repulsive. The structure and mechanical properties of the particle system result from a complex interplay between the particle interaction and the deformation history of the sample. Using mechanical testing and 3D structural analysis of the sample, correlations between particles interaction and the flowability become visible.

CPP 37.14 Wed 15:00 P3

Spatial distributions of surface energies in porous media: Insights from experiments and simulations on the displacement of immiscible fluids — ●JULIE MURISON¹, THOMAS HILLER¹, BENOIT SEMIN^{3,1}, STEPHAN HERMINGHAUS¹, JEAN-CHRISTOPHE BARET¹, MATTHIAS SCHRÖTER¹, and MARTIN BRINKMANN^{2,1} — ¹Max Planck Institute of Dynamics and Self Organisation, Göttingen — ²Experimental Physics, Saarland University — ³Laboratoire de Physique Statistique, ENS, Paris

Various phenomena observed during immiscible displacement in a porous medium can be related to pore wall wettability. Traditionally the overall wettability of a rock sample is quantified by measuring capillary pressure saturation curves (CPS). To establish a link between these global quantities and the pore-scale distribution of surface energies, we developed a series of model porous media with the same average surface energy, but differing in the typical extension of the wettable surface domains. Complementary to the experiments we use multiple particle collision dynamics (MPCD) to simulate two-phase flow in porous media. The MPCD algorithm is extended to allow for different surface energies to create similar model porous media as used in the experiments. Experimental CPS measurements show that the work dissipated in a complete cycle is monotonically decreasing with the size of the heterogeneities. Imaging of the invading liquid fronts using x-ray tomography revealed front smoothing for small correlation lengths, consistent with a dissipation of energy. The same quantitative behavior is observed in the simulations.

CPP 37.15 Wed 15:00 P3

Study of contact lines moving over heterogeneous surfaces — ●TAK SHING CHAN^{1,2}, DANIEL HERDE², and MARTIN BRINKMANN^{1,2} — ¹Universität des Saarlandes, Saarbrücken, Germany — ²Max Planck Institute for Dynamic and Self-Organization, Göttingen, Germany

We study problems of contact lines moving over heterogeneous surfaces using a lubrication model that incorporates dynamics on many length scales from several nanometers, where hydrodynamic slip plays a significant role, to the size of a system with typical dimensions of a few millimeters. We first consider the problem of a time dependent, oscillating microscopic contact angle and derive the essential relation between the amplitudes of the contact line displacement and the amplitude and oscillation frequency of the microscopic contact angle. We also investigate the problem in which a liquid front is driven by external forces to move over a surface with alternating stripes of different wettability on a plane substrate.

CPP 37.16 Wed 15:00 P3

Depinning mechanism of a droplet contact line on a superhydrophobic surface — ●MARCO RIVETTI^{1,2}, ANAÏS GAUTHIER¹, JÉRÉMIE TEISSEIRE¹, and ETIENNE BARTHEL¹ — ¹Surface du Verre et Interfaces, UMR 125 CNRS & Saint-Gobain — ²Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany

It has been demonstrated recently that water droplets on superhydrophobic surfaces may exhibit a strong contact angle hysteresis. Nature offers beautiful examples of both slippery - the lotus leaf - and adhesive - the red rose petal - superhydrophobic surfaces. Several approaches exist in the literature to explain the hysteresis, but most of the models predict the advancing and receding contact angles only under specific hypothesis (i.e. perfect knowledge of the shape of the contact line, given geometry of the surface texture...) In this work we show that the receding motion of the contact line on a textured surface is mediated by the propagation of kinks (step-like defects) all along the perimeter of the drop [1]. We detail the dynamics of this mechanism, and show how the displacement of the contact line and the value of the receding contact angle are affected by the presence of kinks. Our results involve both experiments conducted with water droplets on glass superhydrophobic surfaces and numerical simulations performed with Surface Evolver. We explore the potential of this new concept by assessing the impact of lattice type and texture motive on contact angle hysteresis.

[1] A. Gauthier et al., Phys. Rev. Lett., 110, 046101 (2013)

CPP 37.17 Wed 15:00 P3

Thermal nucleation in ultra thin polymer films on slippery hydrophobic substrates — ●MATTHIAS LESSEL¹, MISCHA KLOS¹, JOSHUA D. MCGRAW¹, OLIVER BÄUMCHEN², and KARIN JACOBS¹ — ¹Saarland University, Experimental Physics, D-66041 Saarbrücken — ²Max Planck Institute for Dynamics & Self-Organization (MPI-DS), D-37077 Göttingen

Spinodal dewetting of thin polystyrene films is subject of many studies

(Seemann et al. PRL 2001, Becker et al. Nat. Mat. 2003). Typically, hydrophilic silicon wafers are used as substrates and a no-slip boundary condition is assumed. Here, we modify silicon wafers with self assembled silane monolayers. The silane substrates provide a slip boundary condition and render the surface hydrophobic. Despite the different surface energy, the hydrophobic coating does not change the long-range van der Waals interactions as compared to hydrophilic silicon wafers. Thus, these systems may dewet spinodally. However, in the experiments, a much higher hole density is observed for hydrophobic wafers than is theoretically expected. We find that the hole density on these substrates is influenced by the dewetting temperature and film thickness. The former leads to the hypothesis of thermal nucleation instead of spinodal dewetting as the hole generating mechanism.

CPP 37.18 Wed 15:00 P3

Forced Displacement Experiments in quasi 2D Porous Media. — ●MICHAEL JUNG^{1,2}, MARTA SANCHEZ DE LA LAMA², 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. Whereas the oil displacement is fairly insensitive to most parameters it shows a pronounced transition depending on wettability. These experimental results are compared to numerical simulations based on multiple particle collisions for analogous pore geometry and wetting conditions.

CPP 37.19 Wed 15:00 P3

Liquid-liquid dewetting — ●STEFAN BOMMER¹, SEBASTIAN JACHALSKI², DIRK PESCHKA², RALF SEEMANN¹ und BARBARA WAGNER² — ¹Saarland University — ²Weierstrass Institute 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. Required experimental input parameters like the ratio of surface tensions of the liquid/air and the liquid/liquid interface and the contact angles which are extracted from the equilibrium shapes of the droplets. The transient droplet shapes are modeled by a lubrication approximation. A remarkable independence of the transient shapes on the start conditions was found theoretically for sufficiently 'mature' droplets which allows for a quantitative comparison with experimental droplet morphologies, whereas both theoretical results describe the experimental results quantitatively.

CPP 37.20 Wed 15:00 P3

Porous hybrid materials structured with breath figure templating — ●ALI HASSAN, VOLKER KÖRSTGENS, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching

Solution casting and spin-coating of polymer solution in volatile solvents can lead to honeycomb-like porous structures if performed under conditions of high relative humidity due to changed wetting conditions. The surface structures known as breath figures are induced by an array of water droplets condensing on the surface without coalescing. In the last stage of the film forming process the water droplets evaporate and a porous structure remains. In this study polyacrylate based thin films are combined with inorganic nanoparticles to obtain hierarchical structured surfaces. The achieved coatings have the potential as a photon scattering functional layer in photovoltaic devices. The films are characterized with UV/vis spectroscopy and the distribution of pores and nanoparticles in the polymer layers is investigated with optical and scanning electron microscopy.

CPP 37.21 Wed 15:00 P3

Interfacial and Wetting Behavior during In-Mold Printing — ●MARTIN DEHNERT¹, EIKE-CHRISTIAN SPITZNER¹, AGNIESZKA KALINOWSKA², MICHAEL GEHDE², ALEXANDER BÖDDICKER³, UTA FÜGMANN³, ARVED CARL HÜBLER³, and ROBERT MAGERLE¹ — ¹Chemische Physik, Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Germany — ²Professur Kunststoffe, Fakultät für Maschinenbau, Technische Universität Chemnitz, Germany — ³Print- und Medientechnik, Fakultät für Maschinenbau, Technische Universität Chemnitz, Germany

In-mold printing enables decoration of plastic parts during injection molding [1]. The image is pad printed onto the surface of the injection mold, the plastic melt is injected, and during solidification and part removal the ink is transferred to the plastic part. The understanding of wetting and adhesion of the ink on the mold and on the plastic part is essential for a successful implementation of this new printing process. We study the involved interfacial phenomena during in-mold printing of polypropylene with optical microscopy, laser scanning microscopy, and atomic force microscopy. The flow patterns of the ink give insight into the physical processes during the ink transfer. We observe different phenomena on the micro- and nanometer scale, such as wetting of the ink on the mold and on the solidified plastic part, as well as adhesion between the ink, the polymer and the mold surface. A Taylor-Saffman instability of the ink indicates the fluid state of the ink and the shrinkage of the polymer during solidification of the plastic part. [1]Härtig T. et al. *Kunststoffe international* 3/2013

CPP 37.22 Wed 15:00 P3

Microemulsion on model surfaces, study of wetting behavior and uptake capacity — ●SALOMÉ VARGAS-RUIZ¹, CHRISTOPH SCHULREICH², ALEXANDRA ABRAHAM¹, MARTIN JUNG³, REGINE V. KLITZING¹, THOMAS HELLWEG², and STEFAN WELLERT¹ — ¹Stranski Laboratory, Technical University Berlin, Str. d. 17.Juni 124, 10623 Berlin, Germany — ²Physical Chemistry III, University Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany — ³Armed Forces Scientific Inst. f. NBC Protection, Humboldtstraße1, 29633 Munster, Germany

We present microemulsion systems as a new and effective cleaning medium for surfaces contaminated with highly toxic organophosphate compounds. The effectiveness of the microemulsions as cleaning agents depends not only on their ability to extract and solubilized the contaminant from the treated area, but also on the initial interactions of these complex fluids and the solid surface. Hence, we study the wetting and uptake processes of microemulsion on model surfaces, constituted by functionalized silicon wafers and porous polymer films of poly(butyl methacrylate-co-ethylene dimethacrylate). It was established that independent of the surface treated, the structure and the concentration of oil in the microemulsion have the major impact on the studied processes. According to the obtained results, we formulate a set of microemulsions able to wet and penetrate surfaces with wide range of chemical nature and morphologies.

CPP 37.23 Wed 15:00 P3

Capillary leveling of stepped perturbations in thin viscous films — ●MARCO RIVETTI¹, THOMAS SALEZ², STEPHAN HERMINGHAUS¹, and OLIVER BÄUMCHEN¹ — ¹Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — ²Laboratoire de Physico-Chimie Théorique, UMR Gulliver 7083 CNRS & ESPCI, Paris, France

Leveling occurs in thin liquid films if the free surface has a non-constant curvature. The consequent flow is driven by local curvature gradients and resisted by viscosity, and it is well described in the lubrication theory through the thin film equation. We here revisit recent developments and present new experiments on the capillary leveling of thin polymer films where the initial non-equilibrium profile is given by a Heaviside function (i.e. a step geometry) [1]. Experimental profiles for several film geometries and molecular weights are measured during relaxation. The leveling is shown to be self-similar, in agreement with theoretical predictions. An analytical solution of the profile has been obtained for small steps, when linearization of the problem is possible [2]. For steps comparable to the thickness of the film we present numerical solutions of the thin film equation which show good agreement with the experiments. We will also discuss the possible transition from leveling to the spreading regime occurring for ultra-thin films.

[1] J.D. McGraw et al., *Phys. Rev. Lett.* **109**, 128303 (2012)

[2] T. Salez et al., *Phys. of Fluids* **24**, 102111 (2012)

CPP 37.24 Wed 15:00 P3

Micro-optical lens array for ultrahigh-throughput fluorescence detection in droplet-based microfluidics — ●JISEOK LIM^{1,2}, PHILIPP GRUNER¹, JEREMY VRIGNON¹, CHRISTOS S. KARAMISTOS², MANFRED KONRAD², and JEAN-CHRISTOPHE BARET¹ — ¹Max Planck Institute for Dynamics and Self-organization, Am Fassberg 17, D-37077 Goettingen, Germany — ²Max Planck Institute for Biophysical Chemistry, Am Fassberg 11, D-37077 Goettingen, Germany

Droplet-based microfluidic systems are promising platforms for high-throughput screening applications. Elementary methods for droplet production, incubation, fusion, and sorting, have been developed over the past years to provide parallelized droplet manipulation required for these applications. Detection systems have so far been poorly parallelized, setting up a bottle neck for the increase of throughput. We demonstrate the design and integration of droplet-based microfluidic devices with microoptical element arrays for enhanced detection of fluorescent signals. We show that the integration of microlenses and mirror surfaces in these devices results in an 8-fold increase of the fluorescence signal and in improved spatial resolution [1]. Finally, we demonstrate that the developed system can be used to detect beta-galactosidase activity of single E.coli cells in 100pL droplets. We reached a throughput more than 100 000 droplets per second, an analytical throughput larger than those obtained using flow cytometry [2]. References: [1] J. Lim et al., Lab Chip, 13, 1472-1475 (2013) [2] J. Lim et al., Appl. Phys. Lett., 103, 203704 (2013)

CPP 37.25 Wed 15:00 P3

Dense Colloidal Suspensions in Microfluidic Flow — ●PHILIPP KANEHL and HOLGER STARK — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin

Dense colloidal suspensions in a pressure driven flow accumulate in the center of the microchannel. Binary mixtures partially demix depending on their densities [1]. In very dense colloidal systems, one observes oscillations in the colloidal flow velocity which is attributed to transient jamming. The oscillations ultimately become irregular when increasing density further [2].

To develop a theoretical understanding of all these effects, we simulate hard disks under pressure-driven flow in two dimensions using the mesoscale simulation technique of Multi-Particle Collision Dynamics which is an efficient particle-based solver of the Navier-Stokes equation.

In our simulations, we reproduce the experimental observations that a binary suspension segregates into its two species. Whereas at equal densities the larger colloids accumulate in the center, this behavior is reversed when smaller colloids are in the majority and reach a critical density. In sufficiently dense, monodisperse suspensions we obtain the observed oscillations in narrow channels. We monitor both fluid and colloidal flow and thereby explore the role of fluid permeation. In addition, in the transient jamming regime we determine the size distribution for the jammed regions and also look for force chains.

[1] D. Semwogererea and E. R. Weeks, *Phys. Fluids*, **20**, (2008).

[2] A. I. Campbell and M. D. Haw, *Soft Matter* **6**, (2010).

CPP 37.26 Wed 15:00 P3

Effect of Wettability on Water-Oil Front Progression in Porous Media — ●ALEN KABDENOV^{1,2}, HAGEN SCHOLL¹, KAMALJIT SINGH^{2,3}, MARCO DI MICHIEL³, 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 progression of a water front forced into an initially oil filled porous medium is explored using ultrafast X-ray tomography. The wettability of the porous media was controlled using different cleaning and coating procedures, different bead material or using different 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. When forcing the water front into a porous media with locally varying wettability the less wettable volumes are bypassed or bridged in the first water flush and are eventually penetrated by water at a late stage of the water flush.

CPP 37.27 Wed 15:00 P3

Influence of monomeric structure on the slip boundary condition of polymeric liquids — ●MISCHA KLOS, SEBASTIAN BACKES, MATTHIAS LESSEL, and KARIN JACOBS — Saarland University, Experimental Physics, D-66041 Saarbrücken

With further miniaturization of microfluidic devices the role of the solid/liquid interface gets more important 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 silicon substrates. On silane surfaces, polystyrene (PS) of low molecular weight shows slip lengths up to micrometers [2]. On AF1600, no significant slip is observable. Recent studies using scattering techniques reveal an ordering of the PS side chains at the solid/liquid interface depending on the structure of the substrate [3]. The situation changes if PMMA or PVP are used: The side groups of PS feature a homogeneous electron environment, yet those of PVP are disturbed by a nitrogen atom, PMMA has no side rings at all. The dewetting experiments show that the slip effect is less pronounced in systems with PVP or PMMA. X-ray scattering methods supplement those findings and give further insight to the slippage mechanism at the solid/liquid interface.[1]O. Bäumchen, et.al., J Phys Condens Matter 24 (2012) 325102 [2]R. Fetzer, et. al, Europhys Lett 75 (2006) 638 [3]P. Gutfreund, et. al.,Phys Rev E 87 (2013) 012306

CPP 37.28 Wed 15:00 P3

Shape and wrinkle analysis of deflated elastic capsules — ●JONAS HEGEMANN, SEBASTIAN KNOCH, and JAN KIERFELD — Department of Physics, Technische Universität Dortmund, 44227 Dortmund, Germany

Elastic capsules, prepared from droplets or bubbles attached to a capillary (as in a pendant drop tensiometer), can be deflated by suction through the capillary. We study this deflation and show that a combined analysis of the shape and wrinkling characteristics enables us to determine the elastic properties in situ. Shape contours are analyzed and fitted using shape equations derived from nonlinear membrane-shell theory to give the elastic modulus, Poisson ratio and stress distribution of the membrane. We include wrinkles, which generically form upon deflation, within the shape analysis. Measuring the wavelength of wrinkles and using the calculated stress distribution gives the bending stiffness of the membrane. We compare this method with previous approaches using the Laplace-Young equation and illustrate the method on polymerized octadecyltrichlorosilane (OTS) capsules. Our results are in agreement with the available rheological data.

CPP 37.29 Wed 15:00 P3

Characterisation of a novel splitting geometry for microdroplets — ●MICHAEL MOSKOPP, MICHAEL HEIN, JEAN-BAPTISTE FLEURY, and RALF SEEMANN — Experimental Physics, Saarland University

For applications in droplet based microfluidics it is essential to manipulate individual droplets. Along with coalescence, sorting and mixing of their contents the splitting of droplets is a crucial basic operation. Besides its employment in practical applications the physical process of droplet pinch off is still not completely understood. The most straight forward way to split droplets is to use channel geometries where they normally break into two parts. We report a novel splitting geometry with a broad main channel which subdivides into three narrow split channels. Thus a droplet is forced to split into three smaller compartments of different volumes along its flow direction. For an experimental study of this geometry the droplet-length and -velocity and the width ratio of the split channels were varied. Several regimes of different splitting characteristics were observed for each channel geometry. At low drop velocities the breakup mechanism is dominated by surface tension and capillary driven relaxation. However at higher flow velocities this relaxation process is negligible. Thus, in this case the splitting can be explained by geometrically cutting the droplet. Understanding droplet splitting in different geometries is crucial for design of future applications.

CPP 37.30 Wed 15:00 P3

Monitoring the Kinetics of Interfacial Polymerizations using Microfluidics — ●INGMAR POLENZ, QUENTIN BROUSSEAU, and JEAN-CHRISTOPHE BARET — Am Fassberg 17, 37077 Goettingen

Interfacial polymerization (IFP) techniques known since the 1960s of

fer a facile route for the rapid production of solid shells along emulsion droplets for the encapsulation of both hydrophilic and hydrophobic ingredients under mild conditions. However, due to the high particle size range gained at common IFP processes still there is a lack of reliable quantitative information on the polymerization kinetics and understanding the governing mechanisms that affect the shell formation and thus the capsule properties.

We use microfluidic PDMS devices for monitoring interfacial polymerization process at emulsion droplets by measuring the interfacial deformation which is induced by a hydrodynamic shear stress caused by consecutively arranged construction chambers. This method allows us to measure the microencapsulation fast-kinetics and precisely compare the reactivity of certain components at the IFP. We study the formation of polyurea microcapsules (PUMCs); shell formation occurs at the oil-water interface by an immediate reaction of amines, dissolved in the aqueous phase, and isocyanates that are dissolved in the oily phase. We find that at the initial shell formation both monomers of this IFP contribute equally to the overall encapsulation rate. We also quantify the retarding effect of surfactants on the encapsulation kinetics. The observations clearly indicate our monitoring device to be a powerful tool for the study of interfacial polymerization kinetics.

CPP 37.31 Wed 15:00 P3

Flow rectification in glass nanopores — NADANAI LAOHAKUNAKORN¹, SANDIP GHOSAL², and •ULRICH F KEYSER¹ — ¹Cavendish Laboratory, University of Cambridge, JJ Thomson Ave, CB3 0HE Cambridge, UK — ²Northwestern University, Evanston, IL60208-3109, USA

Fluid jets are found in nature at all length scales from microscopic to cosmological. Here we report on an electroosmotically driven jet from a single glass nanopore about 75 nm in radius with a maximum flow rate around 15 pL/s. A novel anemometry technique allows us to map out the vorticity and velocity fields that show excellent agreement with the classical Landau-Squire solution of the Navier-Stokes equations for a point jet [1]. We observe a phenomenon that we call flow rectification: an asymmetry in the flow rate with respect to voltage reversal. Such a nanojet could potentially find applications in micromanipulation, nanopatterning, and as a diode in microfluidic circuits.

[1] N. Laohakunakorn, B. Gollnick, F. Moreno-Herrero, D.G.A.L. Aarts, R.P.A. Dullens, S. Ghosal, and U. F. Keyser. *A Landau-Squire Nanojet*. *Nano Letters* 13(11): 5141-6 (2013)

CPP 37.32 Wed 15:00 P3

On the Dynamics of Polymer Brushes — •MICHAEL LANG¹, RON DOCKHORN^{1,2}, MARCO WERNER^{1,2}, TORSTEN KREER¹, and JENS-UWE SOMMER^{1,2} — ¹Leibniz Institute of Polymer Research Dresden, Hohe Straße 6, 01069 Dresden, Germany. — ²Institute of Theoretical Physics, Technische Universität Dresden, Zellescher Weg 17, 01062 Dresden, Germany

We analyze the relaxation dynamics of densely grafted layers of polymer chains under good solvent conditions by Monte Carlo simulations. We find anisotropic monomer mean square displacements when comparing the directions parallel and perpendicular to the grafting plane at intermediate time scales. Our analysis further reveals that the chains relax from the free end towards the innermost monomers. A plateau is observed for the bond-autocorrelation function that grows exponentially in time for the innermost monomers of the brush. Our observations indicate that chain retraction might be the dominating mechanism for the long time relaxation of densely grafted chains.

CPP 37.33 Wed 15:00 P3

Crystallinity Determination of Poly(3-hexyl thiophene) Thin Films by Means of Fast Scanning Calorimetry — •JENS BALKO¹, SOPHIE SEIDEL¹, ANDREAS WURM², CHRISTOPH SCHICK², and THOMAS THURN-ALBRECHT¹ — ¹Institute of Physics, Martin-Luther-University Halle-Wittenberg, 06120 Halle, Germany — ²Institute of Physics, University of Rostock, 18057 Rostock, Germany

Poly(3-hexyl thiophene) (P3HT) is a common polymer semiconductor, often used as material or component in organic field effect transistors or solar cells. The crystallinity of this semicrystalline material is among other parameters governing the electronic mobility. Fast scanning calorimetry allows studying samples with masses ranging from several ng to μg and scanning rates not accessible by conventional DSC. Using the extrapolated reference melting enthalpy of a 100% crystalline material obtained in bulk¹, we determined the crystallinity in thin films of a commercial P3HT. The mass of the thin film samples was determined by calibrating the heat capacity in molten state. The

crystallinity decreases by a factor of 5 starting from the bulk value for thick films down to films having 25 nm thickness. Cooling rate dependent measurements indicate that the reduced crystallinity is not due to a change in crystallization kinetics.

¹ J. Balko et al., resubmitted to *Macromolecules*

CPP 37.34 Wed 15:00 P3

Evidence of random copolymer adsorption at fluctuating selective interfaces from Monte-Carlo simulation studies — •IGOR GAZUZ and JENS-UWE SOMMER — Leibniz-Institut für Polymerforschung Dresden e. V., 01069 Dresden

We performed Monte Carlo simulations of a binary, strongly separated mixture of A- and B-type homopolymers with some amount of random AB copolymers added. We show that the copolymers tend to localize at the interface between A and B species. We also simulated random copolymers in a one-component surrounding and compared the free energy to the case of copolymers at the interface. The result shows that interface adsorption is energetically clearly favored compared to bulk micellization, contrary to the conclusion made in literature. We calculate the reduction of the interface tension due to copolymers and check the theoretical predictions for the adsorption mechanism and scaling laws made in the previous works, where ideal interfaces were considered.

CPP 37.35 Wed 15:00 P3

Influence of Substrate-Solvent Interactions on Strongly Adsorbed Polymer Layers — •DANIEL GEIGER, KIRSTEN DAMMERTZ, MASOUD AMIRKHANI, and OTHMAR MARTI — Institute for Experimental Physics, University of Ulm

Adsorption of poly(methyl methacrylate) (PMMA) on solid substrates forms pseudobrush-like layers. It was found, that even though the adsorption energy of a single chain segment is relatively low, such a layer can be practically irreversibly adsorbed [1] and cannot be removed by rinsing with solvent. Often, e. g. in lithography, such a residual layer is a crucial issue.

We investigated the adsorption of porous monolayers of PMMA on mica and silicon. This enables interaction of the solvent with the substrate leading to a translation and agglomeration as well as partial removal of the polymer on mica. That is not only possible by using the solvent chloroform, but also when using water, in which PMMA is insoluble. Additionally, we observed that annealing has a minor effect on the adsorption strength of such a layer. If applied to a dense layer, washing doesn't cause dewetting or removal of the film.

On silicon substrates movement for both applied liquids is suppressed, but a collapse of single chains was observed when rinsed with water.

[1] P. Frantz and S. Granick, *Kinetics of Polymer Adsorption and Desorption*, *Phys. Rev. Lett.*, 66, 899-902, 1991

CPP 37.36 Wed 15:00 P3

Complex macrophase separated nanostructure induced by microphase separation in lamellar diblock copolymer thin films — JIANQI ZHANG¹, DORTHE POSSELT², KONSTANTINOS KYRIAKOS¹, SEBASTIAN JAKSCH¹, JAN PERLICH³, DETLEF-M. SMILGIES⁴, and •CHRISTINE M. PAPADAKIS¹ — ¹TU München, Physik-Department, Garching — ²IMFUFA, Roskilde University, Denmark — ³DESY, Hamburg — ⁴Cornell University, Ithaca, NY, USA

Complex, macrophase-separated structures in thin films may be prepared from binary blends of diblock copolymers. We have investigated the nanostructures of thin films spin-coated from binary blends of compositionally symmetric poly(styrene-*b*-butadiene) (P(S-*b*-B)) diblock copolymers having different molar masses using atomic force microscopy (AFM) and grazing-incidence small-angle X-ray scattering (GISAXS) after spin-coating and after subsequent solvent vapor annealing. The as-prepared thin films from these binary blends feature mainly perpendicular lamellae in the one-phase state, indicating that the higher molar mass diblock copolymers dominate the lamellar orientation. The lamellar thickness decreases linearly with increasing volume fraction of the low molar mass diblock copolymer. After solvent vapor annealing, well-defined macrophase separated nanostructures appear which feature parallel lamellae near the film surface and perpendicular ones in the bulk.

CPP 37.37 Wed 15:00 P3

PPMA-PMMA block copolymer thin films with modified gold nanoparticles — •DIETER JEHNICHEN¹, DORIS POSPIECH¹,

GUPING HE¹, PETER FRIEDEL¹, JIANQI ZHANG², CHRISTINE M. PAPADAKIS², and JAN PERLICH³ — ¹Leibniz-Institut für Polymerforschung Dresden e.V. — ²Technische Universität München, Physik-Department, Garching — ³DESY Photon Science, Hamburg

Diblock copolymers show phase separation on mesoscopic length scales and form a wealth of ordered morphologies in both bulk and thin films resulting in nanostructured polymer surfaces. These may serve as templates for the controlled assembly of nanoparticles.

We investigate diblock copolymers from poly(*n*-pentyl methacrylate) and poly(methyl methacrylate), P(PMA-*b*-MMA) having different block lengths and compositions. In bulk, they form lamellae or hexagonally packed cylinders [1]. For film thicknesses lower than the repeat distance of the bulk morphology, standing cylinders are observed using atomic force microscopy and grazing-incidence small-angle X-ray scattering. In contrast, for higher film thicknesses, lying cylinders are found. Gold nanoparticles assemble at the interfaces and result in some cases in severe changes of the thin film structure.

1. D. Jehnichen et al., *Z. Kristallogr. Suppl.* **30**, 485 (2009).

CPP 37.38 Wed 15:00 P3

Sensing Adhesion on the Nanoscale - Revealing the Contact Formation of Biomimetic Microstructures — ●JENS W. NEUBAUER¹, JOHANN ERATH¹, DIRK-MICHAEL DROTLEF², ARÁNZAZU DEL CAMPO², and ANDREAS FERY¹ — ¹Universität Bayreuth, Bayreuth, Germany — ²Max-Planck-Institut für Polymerforschung, Mainz, Germany

Evolution has led to various bio-surfaces with specific functionalities. Mimicking the models of nature, the properties of man-made materials can be improved as well. For instance, adhesion can be enhanced by microstructuring of surfaces, as shown for gecko mimicked structures. To understand this effect the stress distribution in the contact area is of special interest.

Therefore, we developed a method for the detection of local contact stresses on biomimetic microstructured surfaces. This mechano-responsive system consists of a fluorescently labeled polymer brush. Its response to pressure loads was calibrated using an atomic force microscope. The brush response is sensitive to low pressures (10 kPa) with a spatial resolution better than human skin (1 μm). Under stress steric interactions arise in the polyelectrolyte brush. We investigated these interactions and compared them with existing polymer brush theories.

Using this polymer-based sensor, we studied the adhesive enhancement of microstructured surfaces combining a commercial setup (PVM-A, GeSim, Germany) with a confocal microscope. Hence, we were able to control the contact formation of the microstructured surface.

CPP 37.39 Wed 15:00 P3

Structure of adhesive-adherent interfaces probed by neutron scattering — ●MARKUS SCHINDLER¹, STEPHAN PRÖLLER¹, THOMAS GEUE², JEAN-FRANCOIS MOULIN³, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str.1, 85748 Garching — ²Laboratory for Neutron Scattering, ETHZ & PSI, 5232 Villigen, Switzerland — ³Helmholtz Zentrum Geesthacht, MLZ, Lichtenbergstr. 1, 85747 Garching

Pressure sensitive adhesives (PSAs) are widely used in everyday applications, industries and medicine. Individually tailored compounds exist for many fields of application. The interactions between an adherent and the polymer adhesive can lead to the establishment of an enrichment layer of one of the PSA's components close the interface. To investigate these buried interfaces neutron scattering is the technique of choice due to its high penetration, e.g. compared with X-rays. We present results from neutron scattering experiments, both TOF-GISANS and neutron reflectivity, revealing the inner structure of the surface-near regions and buried interfaces of a model PSA in contact with an adherent. This model PSA is the statistical copolymer P(EHA-stat-MMA), the adherent of choice is silicon, pre-treated with different cleaning routines. We find very different near-interface enrichment layers for the different buried interfaces.

CPP 37.40 Wed 15:00 P3

Magnetic susceptibility of thin films of ferrocene containing polymers — ●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

We focus on amphiphilic ferrocene block copolymers (here poly(vinyl

ferrocene)-*b*-poly(vinyl pyridin), PVFc-P2VP) and their magnetic susceptibility depending on the oxidation state in thin films. These films are prepared as Langmuir monolayers on a water substrate and as Langmuir-Blodgett multilayer films on a solid silicon substrate. The structure of the films are monitored by X-Ray reflectivity in situ (water subphase) and ex situ (silicon substrate) and analysed in terms of standard models. In the reduced state the structure of the Langmuir monolayers is dominated by the P2VP block partner and strongly ruled by the surface pressure in the monolayer. The oxidised state induces conformational changes of the ferrocene moiety leading to a swelling of the polymer film on solid substrates and to increased solubility in water leading to a collapse of the Langmuir monolayers. Besides the altered structure on solid substrates we find a switching from diamagnetic to paramagnetic susceptibilities (measured by SQUID magnetometry) in dependency on the oxidation ratio of the ferrocene complex. The impact of the degree of order in the multilayer polymer film on the strength of the magnetic response of the thin films will be discussed.

CPP 37.41 Wed 15:00 P3

Salt Induced Reduction of Lysozyme Adsorption at Behenic Acid 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 intracellular and extracellular regions. Many biological processes taking place at membranes are associated with the adsorption of proteins. We present a study on the adsorption behaviour of the protein lysozyme at behenic acid films. In the case of electrostatic interaction between proteins and membranes, the screening effect of salt ions can be used to control the adsorption. Therefore we focus the investigation on the effect of NaCl on the adsorption of lysozyme. By varying the salt concentrations the electrostatic interaction between the positively charged proteins and the negatively charged head groups of the behenic acid is altered resulting in a decreased lysozyme adsorption with rising NaCl concentration. The adsorption process is investigated by x-ray reflectivity measurements, which allow the determination of the electron density profiles of thin layers at the liquid – gas interface.

CPP 37.42 Wed 15:00 P3

Surface Dynamics of Liquid, Thin Polymer Films — ●FAN-YEN LIN, HANS-JÜRGEN BUTT, and WERNER STEFFEN — Max Planck Institute for Polymer Research, P.O. Box 3148, 55128 Mainz, Germany

The emerging technique of resonance enhanced dynamic light scattering (REDLS)[1] was used to study the motions of polymer chains in thin polymer films at different length scales. The polybutadiene (PB) we measured is close to a Newtonian or ideal viscous polymer liquid at room temperature ($T_g+125^\circ\text{C}$). The surface dynamics found can be described by a hydrodynamic capillary wave model[2].

Our studies show the surface dynamics to be strongly suppressed when the length scale is below 25nm. We observe a stiffening behavior decreasing the length scale and by this increasing the confinement. The overall behavior of the dynamics can be explained by a three layer model, bulk behavior in the middle, a more mobile layer at the polymer-air interface and a less mobile layer at the solid substrate-polymer interface.

1, Plum MA, Menges B, Fytas G, Butt HJ, Steffen W, *Rev. Sci Instr.* 2011, 82, 015102

2, Kim H, Rühm A, Lurio LB, Basu JK, Lal J, Lumma D, Mochrie SGJ, and Sinha SK, *Phys. Rev. Lett.* 2003, 90, 068302

CPP 37.43 Wed 15:00 P3

Flexibility investigations on low-temperature processed nanostructured polymer/titania hybrid films — ●TOBIAS WIDMANN, WEIJIA WANG, and PETER MÜLLER BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching

On the way to green energy, hybrid solar cells show great potential. They combine a conducting polymer with an inorganic semiconductor and therefore have advantages of both materials. The flexibility is one of the most promising properties of hybrid solar cells, which ensures the production by a roll-to-roll process and in large scale. Hence, in this work the flexibility of low temperature processed hybrid thin films is investigated. A porous film structure is synthesized by incorporating a titania precursor into a diblock copolymer which functions as the template. Thereafter it is deposited on a flexible substrate and a bending test is implemented by a custom made machine. The alteration of the bare titania structure and the hybrid film structure due to bending

is investigated with optical microscopy and SEM and correlated with photophysical properties probed with UVvis and PL.

CPP 37.44 Wed 15:00 P3

Einfluss der Oberflächensegregation auf die nanomechanischen Eigenschaften von Polystyrol-Polybutadien-Mischungen — ●MARTIN SCHINDLER, MARTIN DEHNERT und ROBERT MAGERLE — Chemische Physik, Fakultät für Naturwissenschaften, Technische Universität Chemnitz, D-09107 Chemnitz, Deutschland

In dünnen Filmen von Mischungen aus Polystyrol (PS) und Polybutadien (PB) Homopolymeren führt die Anreicherung von PB an der Oberfläche von PS-reichen Domänen zu einer Veränderung der nanomechanischen Eigenschaften ihrer Oberfläche. Wir haben dies mittels Multi-Set Point Intermittent Contact mode Rasterkraftmikroskopie untersucht, wobei wir das Volumenverhältnis von PS und PB sowie die Schwingungsamplitude der AFM-Spitze systematisch variiert haben. Die Eindringtiefe der Spitze nimmt auf PS-reichen Bereichen mit zunehmendem PB-Anteil zu, was wir als eine Zunahme der Dicke der PB-Benetzungsschicht an der Oberfläche interpretieren. Bei kleinen Schwingungsamplituden kommt es nur zu einer attraktiven Wechselwirkung zwischen Spitze und Probe und die Kurven der dissipierten Energie weisen sowohl auf PS- wie auch PB-reichen Bereichen der Probe einen parabelförmigen Verlauf auf, der typisch für viskoelastische Materialien ist. Tiefenprofile der effektiven Federkonstante zwischen Spitze und Probe zeigen anschaulich die unterschiedliche Größe der attraktiven und repulsiven Bereiche der Spitze-Probe-Wechselwirkung auf PS und PB reichen Bereichen.

CPP 37.45 Wed 15:00 P3

Stability limits of n-nonane calculated from MD-interface-simulations — ●STEPHAN BRAUN¹, ATTILA IMRE², and THOMAS KRASKA¹ — ¹University of Cologne, Institute of Physical Chemistry, Luxemburger Str. 116, D-50939 Köln — ²HAS Centre for Energy Research, H-1525 POB 49, Budapest

Based on molecular dynamics simulation of the vapor-liquid interface, the classical thermodynamic spinodal for n-nonane is estimated. The determination of the spinodal is based on properties of the liquid vapor interface. This method relates the tangential pressure component through the vapor*liquid interface to the van der Waals loop in the two-phase region of the phase diagram. By application of the thermodynamic stability criteria, the location of the spinodal can be determined. Up to now the applicability of this method was demonstrated for substances such as Lennard-Jones Argon, carbon dioxide or methanol but not for molecules with a highly anisotropic shape. The choice of n-nonane as investigated molecule originates from the question whether a deviation from the spherical symmetry of a molecule affects the prediction of the stability limit data. One might expect that anisotropic properties of the molecules influence the tangential pressure profile and hence the spinodal. As a result, we find that the estimated stability limit data for n-nonane are consistent within the experimental data available for the homologous series of the n-alkanes. It turns out that the slight alignment of the molecules parallel to the interface reported in the literature does not affect the method of transferring interface properties to the bulk phase stability limit.

CPP 37.46 Wed 15:00 P3

Controlling adsorption of semiflexible polymers to planar and curved substrates — ●TOBIAS ALEXANDER KAMPMANN and JAN KIERFELD — TU Dortmund, Germany, NRW

We study the adsorption of semiflexible polymers such as polyelectrolytes or DNA on planar and curved substrates, e.g., spheres or washboard substrates via short-range potentials using extensive Monte-Carlo simulations, scaling arguments, and analytical transfer matrix techniques. We show that the adsorption threshold of stiff or semiflexible polymers on a planar substrate can be controlled by polymer stiffness: adsorption requires the highest potential strength if the persistence length of the polymer matches the range of the adsorption potential. On curved substrates, i.e., an adsorbing sphere or an adsorbing washboard surface, the adsorption can be additionally controlled by the curvature of the surface structure. The additional bending energy in the adsorbed state leads to an increase of the critical adsorption strength, which depends on the curvature radii of the substrate structure. For an adsorbing sphere, this gives rise to an optimal polymer stiffness for adsorption, i.e., a local minimum in the critical potential strength for adsorption, which can be controlled by curvature. For two- and three-dimensional washboard substrates, we identify the range of persistence lengths and the mechanisms for an effective control of the

adsorption threshold by the substrate curvature.

CPP 37.47 Wed 15:00 P3

Influencing optical properties and the morphology in thin polymer films consisting of P3HT, PFO und MEH-PPV by adding small amounts of high-boiling solvent additives — ●MARKUS REICHENBERGER — Universität Bayreuth, Lehrstuhl EP2

If admixing a few volume percent of higher boiling point additives to a solution with constant polymer concentration and solvent, impact on optical transitions, electronic properties and film morphology is resulting. It is shown how this modification of the polymer solution affects thin films of P3HT. The investigation is carried out by different spectroscopical methods and various techniques of surface analysis. Diiodooctane, dichlorobenzene and octanedithiols are used as exemplary high-boiling additives. The effect of incorporating diiodooctane on films made of PFO and MEH-PPV gives approximately equivalent results as in P3HT films: By admixing a small amount of an arbitrary high boiling point additive to the polymer solution, one can control the fraction of amorphous and aggregated phase, hence potentially the charge transport, in the spin-coated polymer film. Many a time in the literature one observes an high energetic peak at 2.12 eV, respectively 585 nm, in the photoluminescence spectrum of thin P3HT films. Recent results are able to clarify the origin of this peak.

CPP 37.48 Wed 15:00 P3

Heteroepitaxial growth of C60 on a substrate: a kinetic Monte Carlo study — ●CHRISTOPHER WÄCHTLER, NICOLA KLEPPMANN, and SABINE H. L. KLAPP — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Thin crystalline fullerite films are currently of high interest as candidates for applications in semiconductor devices. Therefore a good understanding of the growth mechanisms and of the influence of parameters like temperature and the underlying substrate is mandatory.

Experimental data [1] leads us to examine the heteroepitaxial growth of fullerenes on mica. Based on transition state theory and previous studies of C60 epitaxy [2] we use kinetic Monte Carlo simulations to reproduce the experimental results under the same experimental conditions, i.e. temperature, deposition rate and substrate size. In this study we analyze the influence of the substrate on the system dynamics during deposition and subsequent relaxation on a real-space surface on experimental time scales. The systems of lateral extension of 500 to 2000 nm show a Volmer-Weber mechanism and grow near the thermodynamical equilibrium. Morphological quantities such as island density and layer coverage are used to characterize the simulated films. We also investigate the influence of strain on the growth mode of fullerenes grown on a substrate with a lattice constant that is incommensurable to the C60 fcc crystal.

[1] H.-G. Busmann et al., Surf.Sci. 289, 3, (1993).

[2] S. Bommel, N. Kleppmann et al., submitted to PRL

CPP 37.49 Wed 15:00 P3

Nanoparticle distribution and domain orientation in nanoparticle / block copolymer composite thin films — ●ANDRIY HORECHYI¹, BHANU NANDAN², DIETER JEHNICHEN¹, MICHAEL GÖBEL¹, MANFRED STAMM^{1,3}, and DORIS POSPIECH¹ — ¹Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany — ²Department of Textile Technology, Indian Institute of Technology Delhi, New Delhi, India — ³Technische Universität Dresden, Physical Chemistry of Polymer Materials, Dresden, Germany

Block copolymers (BCP) which microphase separate into various morphologies, are widely used as templates for organizing nanoparticles (NP) into 1D, 2D and 3D-periodic structures. In NP/BCP thin films the thermodynamics that governs the BCP morphology becomes more complex as compared to the bulk, mainly due to the interfacial effects that occur at polymer/substrate and/or polymer/air interface.

In this work we studied and compared the effects of chemical composition of BCP on distribution and lateral arrangement of nanoparticles dispersed in BCP thin films, and influence of such nanoparticle-associated effects on the orientation of BCP domains. By changing the chemical composition of BCP constituents, different lateral and orthogonal distributions of nanoparticles are realized. Presence of nanoparticles at polymer/substrate or polymer/air interface changes the effective surface energy and promotes domain re-orientation regardless of whether selective or non-selective NP/polymer interactions are involved. We acknowledge funding by Deutsche Forschungsgemeinschaft (DFG).

CPP 37.50 Wed 15:00 P3

Crystalline and J-aggregated state of semiconducting polymer: thin polycrystalline polyaniline films — NATALIA GOSPODINOVA¹, OLGA OMELCHENKO^{1,2}, ELENA TOMŠÍK¹, and •OLGA GUSKOVA³ — ¹Institute of Macromolecular Chemistry AS CR, Heyrovsky Sq. 2, 162 06 Prague 6, Czech Republic — ²A.N. Frumkin Institute of Physical Chemistry and Electrochemistry RAS, 31 Leninsky prospect, 199071 Moscow, Russian Federation — ³Leibniz Institute of Polymer Research Dresden, Hohe Str. 6, D-01069 Dresden, Germany

Thin polycrystalline polyaniline films according to two dimensional WAXS data are constituted from fibril-like crystals. Full-atomistic molecular dynamics simulation confirms that water-mediated hydrogen bonds are responsible for the self-assembling of aniline oligomers in the fibril direction. Polycrystalline films show a reversible red shift of long-wavelength optical maximum from 570 to 800 nm upon water adsorption. Similarly to dyes long-wave absorption can be attributed to J-like liquid crystalline phase, superficial formation of which is governed by water-mediated intermolecular hydrogen bonding. Thus, a dominating role of hydrogen bonds in crystalline and J-aggregate design of semiconducting polymer has been shown [1].

[1] O. Omelchenko, E. Tomšík, A. Zhigunov, O. Guskova, O. Gribkova, N. Gospodinova // *Macromol. Chem. Phys.* 2013. DOI: 10.1002/macp.201300429.

CPP 37.51 Wed 15:00 P3

AFM Observation of Heterogeneous Nucleation in Epitaxially Crystallized Polymers — ANN-KRISTIN LÖHMANN, •MARTHA SCHULZ, JANA RÜDEL, THOMAS HENZE, and THOMAS THURN-ALBRECHT — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg

We present a microscopic study of heterogeneous nucleation in epitaxially crystallized polymers. Instead of randomly occurring nuclei leading to a spherulitic growth, we find a different mechanism in the case of epitaxy. Crystallization starts from an ordered interfacial layer that is stabilized above the bulk melting point. This layer wets the interface and acts as a nucleus which induces the unusual highly oriented lamellar structure of the crystalline film. Ultrathin films of LLDPE, HDPE and PCL crystallized epitaxially on graphite were studied at temperatures close to the polymer melting point. The AFM measurements at high temperatures were performed in the net-attractive oscillation state [1] of Intermittent Contact Mode. The stabilized interface layer can be found in all of the studied systems with differences in morphology, thickness and stabilized temperature range.

[1] T. Henze, K. Schröter, and T. Thurn-Albrecht, *Nanotechnology* 23, 245702 (2012).

CPP 37.52 Wed 15:00 P3

Automatic, optimized interface placement in Forward Flux Sampling simulations — •KAI KRATZER¹, AXEL ARNOLD¹, and ROSALIND J. ALLEN² — ¹Institute for Computational Physics, University of Stuttgart, Allmandring 3, 70569 Stuttgart, DE — ²SUPA, School of Physics, The University of Edinburgh, Mayfield Road, Edinburgh EH9 3JZ, UK

With Forward flux sampling (FFS) rare events like crystallization phenomena in equilibrium or non-equilibrium systems can be simulated by driving the system from its initial state to the final state via a set of interfaces in phase space. The efficiency as a combination of computational cost and statistical error of FFS depends on the locations of these interfaces. We present two methods for placing the interfaces automatically at optimal locations and on-the-fly during the simulation, without knowledge of the underlying energy landscape of the physical system. Using these methods only the borders of the initial state and the final state in terms of an order parameter must be defined. Then, the simulation finds its own way through phase space by means of inexpensive exploring simulations. This facilitates the setup of an FFS simulations and increases the efficiency of FFS tremendously by placing more interfaces at bottlenecks of the system where the probability of advancement is lower. The method aims at establishing a constant flux through all interfaces, which not only maximizes the efficiency, but also avoids biasing due to bad sampling at interfaces with very low fluxes.

CPP 37.53 Wed 15:00 P3

Micellar solutions of novel thermoresponsive diblock copolymers — •LUKAS AUGSBACH¹, KONSTANTINOS KYRIAKOS¹, ANNA MIASNIKOVA², ANDRÉ LASCHEWSKY², ZHENYU DI³, PETER MÜLLER-BUSCHBAUM¹, and CHRISTINE M. PAPADAKIS¹ — ¹TU München,

Physik-Department, Garching — ²Universität Potsdam, Institut für Chemie, Potsdam-Golm — ³Jülich Centre for Neutron Science, Outstation JCNS, MLZ, Garching

Amphiphilic diblock copolymers with a thermoresponsive block self-assemble into thermoresponsive micelles in aqueous solution. Poly(methoxydiethyleneglycol acrylate) (PMDEGA) is a novel thermoresponsive system, which exhibits cloud points, T_{cp} , in the range 35-45 °C [1]. This system shows peculiar behavior, such as a broad transition region. Moreover, the collapse of the micellar shell has not yet been detected.

Here, we report on small-angle neutron scattering (SANS) experiments on a micellar solution of P(S-*b*-MDEGA) (PS stands for polystyrene) around T_{cp} . The focus is on the structural changes at the cloud point, such as the micellar radius and the correlation of the micelles. At the cloud point, significant structural changes are observed, and the transition occurs over a broad temperature range with intermediate stages, in agreement with previous results on similar PMDEGA systems [2].

[1] A. Miasnikova, A. Laschewsky *J. Polym. Sci. Part A: Polym. Chem.* 2012, **50**, 3313

[2] A. Miasnikova, et al., *Langmuir* 2012, **28**, 4479

CPP 37.54 Wed 15:00 P3

Core-Shell Brush Copolymers with Poly(propylene oxide)-*b*-poly(ethylene oxide) Side Chains — •CHRISTINA PSYLLA¹, KONSTANTINOS KYRIAKOS¹, JUNPENG ZHAO², STERGIOS PISPAS², and CHRISTINE M. PAPADAKIS¹ — ¹TU München, Physik-Department, Garching — ²Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece

Graft copolymers with densely grafted side chains are known as brush copolymers. Brush copolymers with poly(*p*-hydroxystyrene) (PHOS) as the backbone and poly(propylene oxide) (PPO) and poly(ethylene oxide) (PEO) in the side chains, have recently been synthesized and show micelle formation as well as thermoresponsive behavior in aqueous solution [1]. Their multibranch molecular structure may affect their micellization behavior in aqueous solution compared to simple diblock copolymers but also their self-assembly in the bulk.

We report here on small-angle and wide-angle X-ray scattering experiments on several copolymers of various architectures and compositions, carried out in a wide temperature range. In the bulk, significant effects of the chain architecture, i.e. the sequence of PEO and PPO in the side chains and whether the side chains are diblock or random copolymers, and the volume fraction of PPO on the crystalline structure of the PEO block and on the microphase formation are observed.

[1] J. Zhao et al. *Macromolecules* **43**, 1771 (2010)

CPP 37.55 Wed 15:00 P3

Novel thermoresponsive block copolymers of various architectures - a fluorescence correlation spectroscopy investigation of the micelle formation — •KONSTANTINOS KYRIAKOS¹, CHRISTINA PSYLLA¹, SARAH OTTINGER¹, ANNA MIASNIKOVA², ANDRÉ LASCHEWSKY², PETER MÜLLER-BUSCHBAUM¹, and CHRISTINE M. PAPADAKIS¹ — ¹TU München, Physik-Department, Garching — ²Universität Potsdam, Institut für Chemie, Potsdam-Golm

Amphiphilic copolymers with a thermoresponsive block in aqueous solution self-assemble into micelles with a thermoresponsive shell. Poly(methoxy diethylene glycol acrylate) PMDEGA is a new thermoresponsive polymer, which exhibits a cloud point in the range 35-45 °C, i.e. within the most interesting physiological window [1,2]. However, the characteristics of the transition at the cloud point are very different from the ones of the often studied poly(N-isopropylacrylamide) (PNIPAM).

We report here on fluorescence correlation spectroscopy (FCS) experiments on very dilute solutions of various P(S-*b*-MDEGA) block copolymers differing in chain architecture: a diblock, a triblock and a three-arm star copolymer. It was found that, below the cloud point, all three polymers form micelles above the critical micelle concentration (CMC) and have similar hydrodynamic radii.

[1] Miasnikova, A., Laschewsky A. *J. Polym. Sci. Part A: Polym. Chem.* **50**, 3313 (2012)

[2] Miasnikova, A. et al. *Langmuir* **28**, 4479 (2012)

CPP 37.56 Wed 15:00 P3

Influence of the Crystallization Kinetics on the Morphology and Mechanical Properties of Poly- ϵ -Caprolactone —

•ANNE SEIDLITZ¹, YONGFENG MEN², and THOMAS THURN-ALBRECHT¹ — ¹Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Germany — ²State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, China

When a sample is crystallized under isothermal conditions, the crystallization process can be slow (slow regime) or fast (fast regime) compared to the dynamics of the chains in the melt. In the slow regime the chains in the melt should be able to disentangle during crystallization, whereas in the fast regime the chains have no time to dissolve the entanglements. We investigated the influence of the crystallization regime on the morphology and mechanical properties of PCL. We performed tensile measurements in combination with SAXS experiments to investigate the structure and nonlinear mechanical properties. Samples with different molecular weights were isothermally crystallized at different temperatures to reach both regimes. While the morphology is nearly unaffected by the crystallization temperature, we observe a systematic change in the tensile properties, probably caused by a difference in entanglement density between the two crystallization regimes.

CPP 37.57 Wed 15:00 P3

Crystallinity investigations on an aqueous-processable conducting polymer for applications in environmentally friendly organic solar cells — •STEPHAN PRÖLLER^{1,2}, VOLKER KÖRSTGENS², DANIEL MOSEGUÍ GONZÁLEZ², YUAN YAO², SHUN YU³, STEPHAN V. ROTH³, EVA M. HERZIG¹, and PETER MÜLLER-BUSCHBAUM² — ¹TU München, MSE, Lichtenbergstr. 4, 85748 Garching — ²TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching — ³DESY, Notkestr. 85, 22603 Hamburg

When assembling organic solar cells, organic solvents are used which are often even toxic and cause the technology not to be as 'green' as intended to be. Therefore, polymers being processable in non-toxic solvents such as water are of high interest as donor material in the active layer of organic solar cells. One possible polymer is poly[3-(potassium-6-hexanoate)thiophene-2,5-diyl] (P3P6T), a derivative of P3HT. Next to optical properties like absorption and band gap, the crystallinity of polymer films is of special interest in order to obtain efficiently working solar cells. For high charge carrier mobility, local scale ordering appears to be essential. Therefore, detailed studies on the crystallinity of P3P6T and the dependence on annealing temperature are performed. The thin films are prepared via spin coating and solution casting. The optical properties are investigated using UV/Vis spectroscopy. Crystallinity investigations are performed using XRD and GIWAXS measurements.

CPP 37.58 Wed 15:00 P3

Light hinders ordering in polyaniline — ELIZAVETA ALEKSEEVA, ELENA TOMŠÍK, and •NATALIA GOSPODINOVA — Institute of Macromolecular Chemistry AS CR, Heyrovsky Sq. 2, 162 06 Prague 6, Czech Republic

Liotropic liquid crystalline state with features of chromonic mesophase [1] and J-aggregates [2] is shown to precede formation of highly crystalline self-oriented polyaniline films during water evaporation. Importantly, that not only increase of temperature but also exposition to non-polarized light substantially hinders self-assembly into liquid crystalline state which is prerequisite for formation of fibril-like crystals building polycrystalline polyaniline films. X-ray diffraction, optical microscopy and optical absorption spectroscopy have been employed in this study.

[1] J. Lydon, *Liquid Crystals*, 2011, 38, 11-12, 1663-1681, and references therein

[2] S. E. Sheppard, *Rev. Mod. Phys.* 1942, 14, 303.

CPP 37.59 Wed 15:00 P3

Polyaniline as an indicator of the non-clustered water in ionic liquids — •ELENA TOMŠÍK, ELIZAVETA ALEKSEEVA, and NATALIA GOSPODINOVA — Institute of Macromolecular Chemistry AS CR, Heyrovsky Sq. 2, 162 06 Prague 6, Czech Republic

Reversible red-shift of long-wavelength absorption accompanying adsorption of water by thin polycrystalline polyaniline films is considered to be a sign of superficial water-promoted formation of liquid crystalline phase. Moreover, this effect is favored by the presence of highly hydrated ions which destroy clustered water. Such simple optical test has been used by us to detect the presence of the non-clustered water in the ionic liquids. Correlation between structure of anions/cations composed ionic liquid and content of non-clustered water is revealed.

CPP 37.60 Wed 15:00 P3

Diffusion einzelner Polymerkristalle in Polypropylen niedriger Taktizität — •MARTIN NEUMANN, STEFAN KRAUSE und ROBERT MAGERLE — Technische Universität Chemnitz, Chemische Physik, Chemnitz, Deutschland

Elastomeres Polypropylen mit geringer Taktizität hat einen Kristallinitätsgrad von nur 15% und bildet isolierte Kristalle, die in einer amorphen Schmelze eingebettet sind. Rasterkraftmikroskopische Untersuchungen an 60 nm dünnen Filmen liefern mit hoher Ortsauflösung und angemessener Zeitauflösung Bildserien der Veränderungen an der Filmoberfläche. Wir beobachten, dass die isolierten Kristalle nicht ortsfest sind sondern auf Zeitskalen von Stunden und Tagen diffundieren. Aus den Bildserien lassen sich Trajektorien der Kristalle bestimmen, welche Aufschluss über die zu Grunde liegenden Diffusionsprozesse geben. Die Trajektorien können als Translationsdiffusion von Partikeln in einem Flüssigkeitsfilm mit einer Viskosität von $\eta = 10^4$ Pa·s beschrieben werden, die im Bereich der von Polymerschmelzen oberhalb des Glasübergangs bekannten Viskositäten liegt. Die kumulative Verteilung der Diffusionsgeschwindigkeit deutet darauf hin, dass gleichzeitig verschiedenartige Diffusionsprozesse mit unterschiedlichen Diffusionskonstanten stattfinden.

CPP 37.61 Wed 15:00 P3

Comparison of the metastable and the stable phase of eicosane via thermal analysis. — •CARLO DI GIAMBATTISTA, JÖRG BALLER, and ROLAND SANCTUARY — Laboratory for the Physics of Advanced Materials, University of Luxembourg

Upon cooling from the melt eicosane ($C_{20}H_{42}$) exhibits a transition to a metastable orthorhombic phase (rotator I). This metastable phase was investigated by classic Differential Scanning Calorimetry (DSC) and Temperature Modulated DSC (TMDSC). From these measurements thermodynamic quantities as the latent heat of transition and the frequency dependant complex specific heat capacity could be drawn. These were then compared to the stable reference state (trigonal) in the same temperature region. Additional experimental methods (Polarisation Optical Microscopy, X-Ray Diffraction...) were used to get a systematic insight to the processes at hand.

CPP 37.62 Wed 15:00 P3

Monte-Carlo Simulations on the CH_4/CF_4 mixture — JOYJIT CHATTORAJ¹, TOBIAS RISTHAUS², •OLIVER RUBNER¹, STEFAN GRIMME², and ANDREAS HEUER¹ — ¹Institute of Physical Chemistry, University of Münster, Germany — ²Institute of Physical and Theoretical Chemistry, University of Bonn, Germany

It is known, though not understood at all, that methane and perfluoromethane are immiscible below 95K and behave thus similar to other mixtures of hydrocarbons and perfluorinated molecules. In this work we want to study the mixing/unmixing of CH_4/CF_4 in order to unveil the mechanisms that lead to this behaviour.

For the interaction potentials of CH_4-CH_4 , CF_4-CF_4 and CH_4-CF_4 We performed extensive dispersion corrected DFT-calculations which were carefully benchmarked against very accurate CCSD(T) results. These potentials were then approximated by simple spherical potentials (e.g. of the Lennard-Jones type). The approximations were controlled by comparing the experimental structure factor and dynamical properties with Monte-Carlo simulations. We then used different Monte-Carlo-approaches from literature that are well established for studying the mixing/unmixing behaviour of molecular systems to investigate the phase diagram of CH_4/CF_4 at different temperatures. By comparing the results of the DFT-potentials with those of the approximated spherical potentials we were able to determine the influence of the anisotropy of the molecules on the unusual unmixing behaviour of this system.

CPP 37.63 Wed 15:00 P3

Crystallization dynamics of pentanol in silica nanopores — •DANIEL RAU, FABIAN SCHÖN, and ROLF PELSTER — Experimentalphysik, Universität des Saarlandes

We present a dielectric study on the crystallization dynamics of n-pentanol in electrochemically etched porous silica with pore diameters $d_{P1} \approx 7$ nm and $d_{P2} \approx 14$ nm. On slow continuous cooling (< 0.05 K/min), we observed a glass transition instead of crystallization while we find a partial recrystallization upon reheating. This behaviour reflects the different temperature dependences of nucleation and crystal growth. In addition, we studied the crystallization dynamics under isothermal conditions after quenching (≈ 2 K/min) the sample. It is

seen that there is a maximum of the crystallization rate far below the bulk melting point.

CPP 37.64 Wed 15:00 P3

Wang-Landau simulation of polymer melts phase behaviour — ●TIMUR SHAKIROV and WOLFGANG PAUL — Martin Luther Universität, Halle, Deutschland

Phase transitions in polymer melts are under intensive investigation during last years using both theoretical and experimental methods. But Wang-Landau simulations of polymer melts wasn't successive and concerned mainly single chains and dilute systems or lattice models. We present results of off-lattice Wang-Landau simulation of melts of linear semi-flexible chains with stiffens bond potential. Simulated phase behavior of such system corresponds to known results of molecular dynamics simulation and can be estimated for model systems which maximal to minimal number of state ratio is over few thousands of magnitude.

CPP 37.65 Wed 15:00 P3

An improved model for the simulation of patchy particles — ●REINT HIERONIMUS and ANDREAS HEUER — Westfälische Wilhelms-Universität Münster, Institut für physikalische Chemie, Corrensstrasse 30, 48149 Münster, Germany

For the simulation of Janus particles and patchy particles the Kern-Frenkel model is widely used. However, this potential has severe shortcomings since energetically different configurations may yield the same model energy. To improve the potential, we supplemented the energy by an appropriately chosen factor which takes the patch distance into account. Using this potential, we performed Monte-Carlo simulations to investigate the self-assembly of Janus particles in two- and three-dimensional systems. We studied the phase formation depending on parameters such as temperature, density, patch number and patch size. The results were compared to the standard Kern-Frenkel model.

CPP 37.66 Wed 15:00 P3

Vapor-liquid nucleation of water investigated by molecular dynamics simulation — ●MARTIN WAGNER and THOMAS KRASKA — Institute for Physical Chemistry, University of Cologne, Luxemburger Str. 116, D-50939 Köln, Germany

The homogeneous nucleation of water vapor is investigated by molecular dynamics simulation. The investigation of water is of special interest because of the formation of hydrogen bonds which are expected to influence the nucleation. Starting from a homogeneous stable vapor phase the system is super-cooled by quenching in short time. The quench is initialized by changing the kinetic energy of a carrier gas, which then cools down the water system by molecular collisions leading to the onset of water nucleation. From the analysis of the cluster statistics and their development, the nucleation rate as well as the nucleation barrier and the critical cluster size are calculated. Besides regular water also heavy water is investigated and compared to the regular water data. The differences are compared to experimental data for both systems.

CPP 37.67 Wed 15:00 P3

Kinetics of nucleation and crystallization of poly(ϵ -caprolactone) * multiwalled carbon nanotube composites — ●EVGENY ZHURAVLEV¹, ANDREAS WURM¹, PETRA PÖTSCHKE², and CHRISTOPH SCHICK¹ — ¹University of Rostock, Institute of Physics, Rostock, Germany — ²Leibniz Institute of Polymer Research Dresden, Dresden, Germany

The nucleation efficiency of multi-wall carbon nano-tubes (MWCNT) in poly(ϵ -caprolactone) (PCL), as an example, was tested for a wide range of temperatures and cooling rates and compared to the efficiency of homogeneously formed nuclei. The temperature range below the maximum of crystallization rate is generally not accessible for non-isothermal cooling experiments because the sample becomes amorphous at the needed cooling rates. Isothermal experiments after fast quenches extend the temperature range down to and below the glass transition. The employed differential fast scanning calorimeter (DFSC) allows cooling at rates up to 100,000 K/s and precise control of isothermal conditions in the time range from 10⁻⁴ to 10⁴ s. Heterogeneous crystal nucleation dominates at low supercooling, revealing a significant dependence of crystallization rate on MWCNT concentration. No saturation of the nucleation activity at a MWCNT loading of 0.2 to 0.5 wt% was observed. At high supercooling, where homogeneous nucleation is prevalent, the addition of MWCNT does not

enhance neither reduce the crystallization rate. At the temperature of maximum homogeneous nucleation rate, formation of homogeneous nuclei always dominates crystallization.

CPP 37.68 Wed 15:00 P3

In situ Observation of the Ordering Process in Semicrystalline Diblock Co-polymer Thin Films — ●PENG ZHANG¹, GONZALO SANTORO¹, SHUN YU¹, SARATHAL KOYILOTH VAYALLI¹, STEPHAN ROTH¹, and TIANBAI HE² — ¹Deutsches Elektronen-Synchrotron, Notkestraße 85, D-22607 Hamburg, Germany — ²State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, P. R. China

The ordering process allows for explaining the structure transitions during polymer crystallization.¹ However, the absence of the clear illustration of the underlying structure evolution on the nanoscale makes this theory not yet commonly accepted. We address this issue and in situ studied the surface structure evolution of PB-b-PCL diblock copolymer thin films with AFM and microbeam grazing incidence small angle X-ray scattering (GISAXS). We successfully prepared PB-b-PCL thin films with regular microphase structure by thermal treatment.² Then, we in situ studied the underlying structure evolution during crystallization using AFM and GISAXS (PETRA III, DESY) combined with hot stage. GISAXS is a reliable method to in situ study the underlying structure evolution in thin film because of its fast time-resolution ability and statistical relevance.³ We present our in situ results on the ordering process and correlated structure evolution during crystallization.(1)Strobl, G. Eur. Phys. J. E 2000, 3, 165.(2)Zhang, P.; Wang, Z.; Huang, H.; He, T. Macromolecules 2012, 45, 9139.(3)Muller-Buschbaum, P. Anal Bioanal Chem 2003, 376, 3.

CPP 37.69 Wed 15:00 P3

Temperature dependent crystallization of iPP: a combined SIST-AFM study — ●LISA UBERLACKER, THOMAS FISCHINGER, and SABINE HILD — Institute of Polymer Science, JKU, Linz, Österreich

The crystallization process of semi-crystalline polymers can be divided in three stages: nucleation, growth and perfection of the crystal structure. At homogeneous and/or heterogeneous nuclei the polymer chains begin to organize and are folding in parallel segments, so called lamellae. The growth occurs radially and results finally in spherulites. This structure formation especially the thickness and perfection of lamellae is influenced strongly by temperature. Stepwise isothermal segregation technique (SIST) is a suitable method to determine the perfection of the lamellae - forming und thickening - during various temperature stages of semi-crystalline polymers like isotactic polypropylene. The method requires several isothermal crystallization steps. Isotactic polypropylene samples with different molecular weight distributions were examined with five isothermal crystallization steps in a range from 145°C to 105°C. The obtained melting endotherms were converted in lamellae thickness distributions using the Gibbs-Thomson equation. For validation the lamellar thicknesses were determined by scanning force microscopy. The comparison between samples with different molecular weight distribution (MWD) and crystallization temperatures show that samples with broader MWD form thinner lamellae than in the samples with smaller MWD. Determine the influences of the single crystallization temperatures on the lamellae forming higher crystallization temperatures obtain thinner lamellae

CPP 37.70 Wed 15:00 P3

First order phase transition at Random Close Packing of spheres — ●FRANK RIETZ¹, CHARLES RADIN², HARRY L. SWINNEY³, and MATTHIAS SCHRÖTER¹ — ¹Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Goettingen, Germany — ²University of Texas at Austin, Department of Mathematics — ³University of Texas at Austin, Center for Nonlinear Dynamics

The name Random Close Packing refers to the experimental observation that some ways of packing of monodisperse beads (like vertical vibration or sedimentation) cannot exceed a volume fraction of about 64%. There are several competing theories for this phenomenon. However, it is possible to surpass the random close packing limit by cyclic shearing [1]. We investigate the three-dimensional distribution of particles in such a shear cell. Below the Random Close Packing density the packing compacts by reconfiguring particles in denser but disordered arrangements. At Random Close Packing the compaction process saturates involving all particles in tetrahedral-like configurations. These structures are locally dense however compose not the maximum global density that is achievable for spheres. Further increase of the den-

sity is only possible by large-scale bead rearrangements that lead to crystalline nuclei and ordered particle ensembles. From the distribution of local volumes around every sphere a first order phase transition is observed. The transition is visible in the polytetrahedra network, angular order parameter, local clusters, and Voronoi shapes.

[1] Nicolas; Eur. Phys. J. E 3, 309 (2000).

CPP 37.71 Wed 15:00 P3

Tagged Chain Rotational Dynamics of Segments in Entangled Polymers — ●MARIE-LUISE TRUSCHEL, ANTON MORDVINKIN, and KAY SAALWÄCHTER — Institut für Physik - NMR, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

We used simple NMR techniques to probe the dynamics of entangled polymer chains. We measured the orientational autocorrelation function (OACF) for different molecular weights of polybutadiene (tagged chain) in bulk and diluted in deuterated matrix of polymers of variable molecular weight in order to investigate the influence of constraint release processes. Earlier work concentrated on the dynamics in regime II-IV [1, 2, 3], while an extension of our technique allows us to reach regime I. The transition from regime I to II will be studied and compared with the value of τ_e known from theory.

[1] Vaca Chávez, Saalwächter, PRL 104, 198305, 2010.

[2] Vaca Chávez, Saalwächter, Macromolecules 44, 1549-1559, 2011

[3] Furtado et al., Macromolecules, 2014, DOI: 10.1021/ma4021938

CPP 37.72 Wed 15:00 P3

Determining the stereochemistry and key excitations in the CD spectra of organic molecules by theoretical methods — ●ZLATKO BRKLJAČA¹, DAVID M. SMITH^{2,3}, and ANA-SUNČANA SMITH^{1,2} — ¹Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Erlangen, Germany — ²Institute Ruđer Bošković, Zagreb, Croatia — ³Computer Chemie Centrum, Universität Erlangen-Nürnberg, Erlangen, Germany

Circular dichroism (CD) spectroscopy is one of the most useful methods for the determination of the absolute configuration of optically active molecules, which is one of the key aspects of molecular stereochemistry. However, since the CD spectrum very strongly depends on the molecular flexibility of the chromophores, the interpretation

of the experimental data is challenging, and hence theoretical modelling is necessary to properly assign the absolute configurations. In a recent study we have shown that a combination of replica exchange molecular dynamics, clustering procedure, and TD-DFT methods can provide a general framework for the calculation of the CD spectra of flexible molecules. We find that successful modelling of CD spectra requires systematic treatment of the solvent induced polarisation. We validate our methodology by finding excellent agreement with the experimental spectra of 3 novel compounds, namely rhodomirtals 1–3, for which we successfully determine the absolute configurations. We furthermore apply our method to flexible peptides and explore how the predominant amide and aromatic excitations shape the overall result.

CPP 37.73 Wed 15:00 P3

Interaction of semiflexible filamentous virus particles with freestanding lipid membranes — ●ANASTASIA B. ARTEMIEVA, PETERA SCHWILLE, and EUGENE P. PETROV — Max Planck Institute of Biochemistry, 82152 Martinsried, Germany

Recently, an unexpected phenomenon [1] of membrane-driven coil-globule transition of DNA macromolecules electrostatically adsorbed to strongly charged freestanding cationic lipid bilayers [2] has been observed experimentally. To elucidate the effect of the polyelectrolyte persistence length in membrane-driven polyelectrolyte condensation, we study the behavior of much stiffer semiflexible *fd* virus particles ($l_p \sim 2.2 \mu\text{m}$) electrostatically adsorbed on freestanding cationic lipid membranes. At low membrane charge densities, membrane-adsorbed *fd* virus particles behave as semiflexible filaments in 2D. However, at higher membrane charge densities, membrane-driven interactions are strong enough to induce the membrane-driven collapse of the relatively stiff *fd* virus particles, which agrees with the predictions of the recent theory of membrane-driven polyelectrolyte condensation [3]. Further, for *fd* virus particles adsorbed at higher surface densities on weakly charged membranes we observe a new effect of membrane-driven self-organization of the virus particles into long linear chain aggregates.

[1] C. Herold, P. Schwille, and E. P. Petrov, *Phys. Rev. Lett.* **104** (2010) 148102.

[2] C. Herold, G. Chwastek, P. Schwille, and E. P. Petrov, *Langmuir* **28** (2012) 5518.

[3] A. G. Cherstvy and E. P. Petrov, *PCCP* (2014) in press.

CPP 38: Focused Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale V (original: O, joined by CPP)

Time: Wednesday 16:00–19:15

Location: TRE Ma

Topical Talk

CPP 38.1 Wed 16:00 TRE Ma

Theory of nonlinear phonics for coherent light-control of solids — ●ANTOINE GEORGES^{1,2,3}, ALASKA SUBEDI², and ANDREA CAVALLERI⁴ — ¹College de France, Paris, France — ²Ecole Polytechnique - CPHT, Palaiseau, France — ³University of Geneva, DPMC, Switzerland — ⁴Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

The use of light to control the structural and electronic properties of solids is an area of great current interest. We present a microscopic theory [arXiv:1311.0544] for ultrafast control of solids with high-intensity Tera-Hertz frequency optical pulses. When resonant with selected infrared-active vibrations, these pulses transiently modify the crystal structure and lead to new collective electronic properties. The theory predicts the dynamical path taken by the crystal lattice using first-principles calculations of the energy surface and classical equations of motion, as well as symmetry considerations. Two classes of dynamics are identified. In the perturbative regime, displacements along the normal mode coordinate of symmetry-preserving Raman-active mode can be achieved by cubic anharmonicities. This validates the mechanism proposed by Först et al. [Nature Physics 7, 854 (2011)] and explains the light-induced insulator-to-metal transition of manganites reported experimentally by Rini et al. [Rini et al. Nature 449, 72 (2007)]. We also predict a new non-perturbative regime in which ultra-fast instabilities that break crystal symmetry can be induced.

CPP 38.2 Wed 16:30 TRE Ma

DFT+Frontier Orbital U — ●EMINE KUCUKBENLI and NICOLA MARZARI — Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne (CH)

Piecewise linearity of the total energy with respect to occupations is not only a fundamental property that should be obeyed by any exact energy functional, but also a starting point to improve approximate functionals that are used in practical applications.

DFT+U enforces piecewise linearity on the Hubbard manifold [1], and it has been shown to greatly improve the accuracy of density-functional theory for transition-metal complexes, thanks to its correction of self-interaction errors [2]. However, it still performs poorly in complexes where significant covalency is present, and intersite corrections (so-called DFT+U+V) have been introduced to improve these challenging cases [3].

Here, we revisit piecewise linearity within the DFT+U and DFT+U+V correction schemes, and explore a novel approach where self-interaction corrections are applied directly to the frontier orbitals. We test this approach on model transition metal complexes, where highly accurate reference results can be established, and on small molecules with varying degrees of covalency.

References: [1] M. Cococcioni and S. de Gironcoli, *Phys. Rev. B* **71**, 35105 (2005). [2] H. J. Kulik, M. Cococcioni, D. A. Scherlis and N. Marzari, *Phys. Rev. Lett.* **97**, 103001 (2006). [3] V. Leiria Campo Jr and M. Cococcioni, *J. Phys. Cond. Matt.* **22**, 055602 (2010); H. J. Kulik and N. Marzari, *J. Chem. Phys.* **134**, 094103 (2011).

CPP 38.3 Wed 16:45 TRE Ma

Quasiparticle self-consistent GW method with spin-orbit coupling applied to Bi and HgTe — ●CHRISTOPH FRIEDRICH, IRENE AGUILERA, MARKUS BETZINGER, and STEFAN BLÜGEL — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We present an implementation of the quasiparticle self-consistent (QS) GW method where the spin-orbit coupling (SOC) is fully taken into account in each iteration rather than being added *a posteriori*. The implementation is based on the FLAPW method. The SOC gives rise to spin off-diagonal blocks in the Green function G^{SOC} and the self-energy $\Sigma^{\text{SOC}} = iG^{\text{SOC}}W^{\text{SOC}}$. We applied the $QSG^{\text{SOC}}W^{\text{SOC}}$ method to the semimetal Bi, which presents in experiment small electron and hole pockets and a tiny band gap (11-15 meV) at the L point, all of them largely overestimated by LDA (e.g., the gap is 86 meV). The $QSG^{\text{SOC}}W^{\text{SOC}}$ approach predicts a value of the band gap of 8 meV and electron and hole pockets in very good agreement with experiment. The *a posteriori* treatment of the SOC ($QSGW+\text{SOC}$), on the other hand, yields an unphysical result for Bi, predicting it to be a topological insulator with a very large gap at L (260 meV) instead of a trivial semimetal. Similarly, for HgTe, $QSGW+\text{SOC}$ reorders the bands in a wrong way and opens a gap at the Γ point in disagreement with experiment. In contrast, the $QSG^{\text{SOC}}W^{\text{SOC}}$ approach yields a qualitatively and quantitatively correct description of the electronic band structure. We acknowledge support from the Helmholtz Association through the Virtual Institute for Topological Insulators (VITI).

CPP 38.4 Wed 17:00 TRE Ma

Studies of semiconducting pyrite and marcasite compounds using many-body perturbation theory in the GW approximation — ●TIMO SCHENA, GUSTAV BIHLMAYER, CHRISTOPH FRIEDRICH, and STEFAN BLÜGEL — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, Germany

FeS₂ pyrite and marcasite have recently gained renewed interest as materials for photovoltaic applications, due to their large optical absorption and abundance. Therefore, a reliable description of the fundamental band gap of these compounds within first-principles calculations is desirable. However, common density functional theory (DFT) often suffers from an underestimation of band gaps. This calls for beyond-DFT methods, e.g., the GW approximation, which is known to yield gaps in much better agreement with experiment. Although this is widely accepted for “simple” semiconductors, the situation is not well understood for more complicated cases, where the band edges differ in atomic and orbital character. In fact, we observe an uncommon band gap reduction in FeS₂ when applying single-shot GW on top of DFT, which might be problematic for photovoltaic applications [1]. In this work, we investigate the effects of the GW approximation on a couple of pyrite and marcasite compounds, employing the FLAPW code FLEUR and the GW code SPEX (www.flapw.de). In addition to single-shot GW , we also compare to the results of the recently implemented quasi-particle self-consistent GW approximation. We gratefully acknowledge funding from BMBF of the NADNuM project 03SF0402A.

[1] T. Schena *et al.* Physical Review B (accepted 2013)

15 min. break

CPP 38.5 Wed 17:30 TRE Ma

Probing d-band Quantum Well States in Palladium Nanofilms — ●SRIJAN KUMAR SAHA¹, SUJIT MANNA¹, MAREK PRZYBYLSKI^{1,2}, VALERI STEPANYUK¹, and JURGEN KIRSCHNER^{1,3} — ¹Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — ²Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, 30-059 Kraków, Poland — ³Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

We present the results of our new study which probes the d-bands quantum well (QW) states in Pd nanofilms grown on Cu(001) using first-principles density functional theory (DFT) calculations combined with scanning tunneling spectroscopy (STS) experiments. This study reveals that QW states occur in the overlayer films of Pd over a strikingly large film thickness (up to 17 monolayers) and in a large binding energy range (from 0.1 to 3.0 eV below Fermi level), thanks to its distinct and broad 4d-bands. The orbital characters of these states are unambiguously identified by our DFT calculations. Calculations also demonstrate oscillatory multilayer relaxations and d-derived quantum size oscillations in Pd films. The pseudomorphic growth, well-defined interface, and spatially resolved STS allows us to probe individual occupied QW states and extract the accurate dispersion of the (Δ_5 -like) d electronic band, as these states are laterally highly localized and give rise to distinct and sharp feature in the tunneling spectra.

CPP 38.6 Wed 17:45 TRE Ma

Implementation and analysis of a plane wave and real space

pseudopotential method including an efficient spin-orbit coupling treatment tailored to calculate the electronic structure of large-scale semiconductor nanostructures — ●FRANK ZIRKELBACH, PIERRE-YVES PRODHOMME, JEROME JACKSON, and GABRIEL BESTER — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

The implementation of the *large-scale atomic effective pseudopotential program* to solve the Schrödinger equation of an electronic system is discussed. *Atomic effective pseudopotentials* that are derived from screened local effective crystal potentials of self-consistent density functional theory (DFT) calculations are utilized, which ensure an accurate treatment at reduced computational costs. The capability of describing relevant electronic eigenstates of a quantum dot structure consisting of hundred thousand atoms at an atomistic *ab initio* level comparable to DFT is demonstrated. The possibility to represent the wavefunction and to evaluate parts of the Hamiltonian either in a plane wave or real space basis allows for a coherent analysis of various different approaches. In the fully real space treatment, linear scaling with respect to the system size is achieved. The convergence behavior of the different methods and utilized approximations is shown. Furthermore, an efficient spin-orbit treatment different to previously existing implementations within the pseudopotential formalism is outlined. The accuracy of the method is demonstrated via direct comparison to standard DFT codes.

CPP 38.7 Wed 18:00 TRE Ma

Strong Parallelization of Real-Space DFT Calculations — ●ANDREA NOBILE^{1,2}, PAUL BAUMEISTER^{1,2}, DANIEL WORTMANN¹, and STEFAN BLÜGEL¹ — ¹Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — ²Jülich Supercomputing Center, Forschungszentrum Jülich, 52425 Jülich, Germany

The rapid change in modern supercomputing architectures poses a challenge to well established DFT codes. In particular, the increase in raw floating point power obtained through parallelism at different levels is not easily exploitable by using the traditional direct diagonalization methods. We will present our new real-space Projector Augmented Wave (PAW) implementation. The real-space representation of the wave functions, densities and potentials, enables the usage of very flexible boundary conditions and naturally adapts to massively parallel architectures. Parallelism can be exploited in the form of domain decomposition of the three dimensional grid, k-point sampling and bands. The kinetic energy operator, realized as a finite difference stencil, is localized. As a consequence the real-space representation of the Hamiltonian is sparse. This limits the amount of necessary communications and allows an application of the operator to a trial vector in order(N) operations. We will present results about the efficiency of the most numerical intensive parts of the code and we will compare the accuracy of the calculations for reference systems with other established DFT methods.

CPP 38.8 Wed 18:15 TRE Ma

Rare Earth Metals in Density-Functional Theory — ●MARCO CASADEI¹, XINGUO REN², PATRICK RINKE¹, ANGEL RUBIO^{1,3}, and MATTHIAS SCHEFFLER¹ — ¹Fritz-Haber-Institut der MPG, Berlin — ²University of Technology, Hefei, China — ³NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

The presence of f electrons in the rare earths and their interaction with the s and p electrons give rise to several physical phenomena. One prominent example is the isostructural α - γ phase transition in cerium (Ce). We have shown that density-functional theory (DFT) captures the volume collapse associated with the transition, but only if advanced functionals such as exact exchange plus correlation in the random-phase approximation (EX+cRPA) are used [1]. The volume collapse is understood in terms of a *localization/delocalization* of the f electrons. We then addressed the question: *is the isostructural volume collapse in cerium unique?* By applying DFT, we studied lanthanum (La), praseodymium (Pr) and neodymium (Nd), which undergo several structural changes with pressure. We find that the transitions are already captured at a lower level of DFT (i.e. with (semi)-local functionals) and therefore conclude that f -electrons are not the driving force in this case. Within hybrid functionals, we find only one phase in lanthanum, which has no f -electrons, and more than one stable solution in the fcc crystal for Pr and Nd, as found for Ce. Unlike in Ce, however, there is always one solution that is the most stable, thus no isostructural volume collapse emerges in agreement with experiments. [1] M. Casadei *et al.*, Phys. Rev. Lett. **109**, 14642 (2012).

CPP 38.9 Wed 18:30 TRE Ma

Electronic Structure and van der Waals Interactions in the Stability and Mobility of Point Defects in Semiconductors — •WANG GAO and ALEXANDRE TKATCHENKO — Fritz-Haber-Institut der MPG, Berlin, Germany

Point defects are abundant in materials, and significantly affect the electronic, optical, and magnetic properties of solids. However, our understanding of the stability and mobility of point defects remains incomplete, despite decades of intensive work on the subject. In the framework of density-functional theory, Perdew-Burke-Ernzerhof functional underestimates formation energies by 0.7 eV due to the electron self-interaction error, while Heyd-Scuseria-Ernzerhof (HSE) functional yields formation energies in better agreement with high-level many-body methods, but often overestimates migration barriers by up to 0.4 eV.

Using HSE coupled with screened long-range vdW interactions [1], we demonstrate that HSE+vdW can simultaneously and accurately describe the formation energies and migration barriers of point defects. The inclusion of vdW interactions significantly changes the transition state geometries, and brings migration barrier into close agreement with experimental values for six different defects. For multiatom vacancies and point defects in heavier semiconductors, vdW interactions play an increasingly larger role [2].

[1] G. X. Zhang, *et al.*, PRL **107**, 245501 (2011); A. Tkatchenko, *et al.*, PRL **108**, 236402 (2012).

[2] W. Gao and A. Tkatchenko, PRL **111**, 045501 (2013).

CPP 38.10 Wed 18:45 TRE Ma

Scaling Laws for van der Waals Interactions in Nanostructured Materials — •VIVEKANAND GOBRE and ALEXANDRE TKATCHENKO — Fritz Haber Institut der MPG, Berlin

Accurate description of van der Waals (vdW) interactions is crucial for precise prediction of structure and stability of complex materials. VdW forces originate from interactions between fluctuating multipoles in matter and play a significant role in the self-assembly of nanostruc-

tured materials. Many models used to describe vdW interactions in nanomaterials are based on a simple pairwise-additive approximation, neglecting the strong electrodynamic response effects caused by long-range fluctuations in matter. We develop and utilize an efficient microscopic method [1,2] to demonstrate that vdW interactions in nanomaterials act at distances greater than typically assumed, and can be characterized by different scaling laws depending on the dimensionality and size of the system. Specifically, we study the behaviour of vdW interactions in single-layer and multilayer graphene, fullerenes of varying size, single-wall carbon nanotubes and graphene nanoribbons. As a function of nanostructure size, the van der Waals coefficients follow unusual trends for all of the considered systems, and deviate significantly from the conventionally employed pairwise-additive picture. We propose that the peculiar van der Waals interactions in nanostructured materials could be exploited to control their self-assembly. [1] Tkatchenko, DiStasio, Car, and Scheffler, PRL (2012); [2] Gobre, Tkatchenko, Nat. Commun. (2013).

CPP 38.11 Wed 19:00 TRE Ma

2D nanopatterns of shape-persistent molecular polygons on HOPG — •STEFAN-S. JESTER, NINA SCHÖNFELDER, EVA SIGMUND, and SIGURD HÖGER — Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Shape-persistent organic molecules with flexible side chains self-assemble at the solution/solid interface to form 2D nanoarchitectures. Scanning tunneling microscopy yields a submolecularly resolved insight into the adsorbate structures. A key issue is how the shape and symmetry of the backbones and their alkyl chain substitution pattern determine the shape and symmetry of the adsorbate patterns. Recently we focused on molecular polygons (triangles, squares, pentagons, and hexagons) with dithiophene corners and phenylene-alkynylene sides.[1] In my talk I will give insight into the relation between Archimedean surface patterns and supramolecular 2D adlayers. [1] S.-S. Jester, E. Sigmund, S. Höger *J. Am. Chem. Soc.* **2011**, *133*, 11062.

CPP 39: Active Colloids

Time: Thursday 9:30–11:00

Location: ZEU 260

Invited Talk

CPP 39.1 Thu 9:30 ZEU 260

Clustering and phase separation of repulsive self-propelled discs — •THOMAS SPECK — Institut für Physik, Johannes Gutenberg-Universität Mainz, 55128 Mainz

A striking non-equilibrium phenomenon is the clustering of phoretically propelled colloidal particles due to the interplay of volume exclusion and persistence of motion. I will review recent experimental results and present first steps towards a microscopic theory for active Brownian particles without alignment. Starting from the many-body Smoluchowski equation in two dimensions, an effective evolution equation of the tagged particle density is derived. Even for purely repulsive disks, this equation reveals a dynamical instability corresponding to a mobility-induced phase transition. This instability leads to the phase separation of the suspension into a dilute gas phase of single active particles, and a single large cluster. The analytical results are corroborated by extensive numerical simulations for different repulsive pair potentials.

CPP 39.2 Thu 10:00 ZEU 260

Gravitaxis of asymmetric microswimmers — •FELIX KÜMMEL¹, BORGE TEN HAGEN², RAPHAEL WITTKOWSKI³, HARTMUT LÖWEN² and CLEMENS BECHINGER^{1,4} — ¹Physikalisches Institut, Universität Stuttgart, Germany — ²Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Germany — ³SUPA, School of Physics and Astronomy, University of Edinburgh, United Kingdom — ⁴Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany

Micron-sized self-propelled colloidal particles can serve as models for real biological swimmers [1]. For giving better insight into the swimming properties of biological microorganisms with an asymmetric shape, we recently studied the motional features of L-shaped microswimmers under bulk conditions [2]. However, most motile objects additionally respond to an external gravitational field, a phenomenon called gravitaxis. For many flagellates and ciliates, such as *Chlamydomonas*

or *Paramecium*, negative gravitaxis has been observed, i.e. a swimming motion opposed to the gravitational field. Such a behavior often originates from an inhomogeneous mass distribution, which aligns the cell similar to a buoy. In contrary, we study the motion of asymmetric L-shaped microswimmers with homogeneous mass distribution, in the presence of a gravitational force. In experiments and by theoretical modeling we demonstrate that a shape anisotropy alone is sufficient to induce gravitactic motion. [1] G. Volpe, *et al.*, *Soft Matter* **7**, 8810 (2011). [2] F. Kümmel, *et al.*, *Phys. Rev. Lett.* **110**, 198302 (2013).

CPP 39.3 Thu 10:15 ZEU 260

Alignment of active particles with hydrodynamic interactions and formation of a self-assembled pump — MARC HENNES, •KATRIN WOLFF, and HOLGER STARK — Institut für Theoretische Physik, Technische Universität Berlin

Hydrodynamically interacting active particles in an external harmonic potential are known to form a self-assembled pump at large enough Peclet numbers [1]. Here, we give a quantitative criterion for the formation of the pump for active Brownian particles depending on the rotational diffusion of particles, their swim speed and the strength of the harmonic trap. The emerging flow field caused by the swimmers corresponds to a regularized stokeslet and stabilises the pump. We find that the particle distribution settles into a non-equilibrium steady state with non-vanishing flux. The particle orientations can be mapped onto an equilibrium system as they align along a common "pump axis" in analogy to dipoles in an electric field. We perform Brownian dynamics simulations with hydrodynamic interactions and compare the many-particle simulations with an analytically tractable mean field system.

[1] R. W. Nash *et al.*, *Phys. Rev. Lett.* **104**, 258101 (2010)

CPP 39.4 Thu 10:30 ZEU 260

Size dependent efficiency of optically heated Janus Particles. — •ANDREAS BREGULLA and FRANK CICHOS — Universität Leipzig,

Deutschland

For nanoscale manipulations in liquids Brownian motion is a limiting factor. In nature various transport mechanisms have evolved which overcome the Brownian fluctuations. Recently, a number of model swimmers have been fabricated and shown to provide similar function. However, hardly no detailed experimental study of their swimming efficiency exists. Here we investigate experimentally the efficiency of self-propelled photophoretic swimmers based on metal-coated polymer particles of different size. The metal hemisphere absorbs the incident laser power and converts its energy into heat, which dissipates into the environment. A phoretic surface flow arises from the temperature gradient along the particle surface and drives the particle parallel to its symmetry axis. Scaling the particle size from micro to nanometers the efficiency of converting optical power into motion is expected to rise with the reciprocal size for ideal swimmers. However, due to the finite size of the metal cap, the efficiency of a real swimmer reveals a maximum depending sensitively on the details of the metal cap shape. We compare the experimental results to numerical simulations.

CPP 39.5 Thu 10:45 ZEU 260

Non-Gaussianity in suspensions of self-propelled Janus particles — ●BORGE TEN HAGEN¹, XU ZHENG², ANDREAS KAISER¹,

ZHANHUA SILBER-LI², and HARTMUT LÖWEN¹ — ¹Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany — ²State Key Laboratory of Nonlinear Mechanics, Institute of Mechanics, CAS, Beijing 100190, People's Republic of China

Spherical Janus particles are one of the most prominent examples for active Brownian objects. Here, we study the diffusiophoretic motion of such microswimmers in experiment and in theory. Three stages are identified: simple Brownian motion at short times, super-diffusion at intermediate times, and finally diffusive behavior again at long times. These three regimes observed in the experiments are compared with a theoretical model for the Langevin dynamics of self-propelled particles with coupled translational and rotational motion. Besides the mean square displacement also higher displacement moments are addressed. In particular, theoretical predictions regarding the non-Gaussian behavior of self-propelled particles are verified in the experiments. The non-Gaussianity is also clearly manifested in the displacement probability distribution of the Janus particles. In agreement with Brownian dynamics simulations, either an extremely broadened peak or a pronounced double-peak structure is found depending on the experimental conditions.

CPP 40: Colloids and Complex Liquids III

Simulation/Theory

Time: Thursday 11:15–12:45

Location: ZEU 260

CPP 40.1 Thu 11:15 ZEU 260

Dynamical signatures of length-scale dependent hydrophobic hydration — ●RICHARD GREGOR WEISS¹ and JOACHIM DZUBIELLA^{1,2} — ¹Humboldt Universität zu Berlin — ²Helmholtz-Zentrum Berlin

We present an investigation of the curvature dependence of water dynamics at hydrophobic solutes by using Molecular Dynamics simulations of SPC/E water at differently sized spherical model surfaces.

As an important novel insight into the subject we present the dependence of water molecule mobility on surface curvature. The findings show that the diffusional behavior and the sojourn times of water molecules at hydrophobic surfaces strongly depend on surface curvature. In addition the curvature dependence exhibits a non-monotonic progression as it is already known for water hydration structure [1].

Our study demonstrates the existence of an intimate connection between static and dynamic curvature effects of hydrophobic hydration. Large implications arise for the interpretation of dynamical measurements of hydration at heterogeneous biomolecular surfaces with varying surface geometry.

[1] D. Chandler, vol. 437, pp 640-647, Nature

CPP 40.2 Thu 11:30 ZEU 260

Alignment of cylindrical colloids induced by critical Casimir torques — ●MARCEL LABBÉ-LAURENT^{1,2}, MATTHIAS TRÖNDLE^{1,2}, LUDGER HARNAU^{1,2}, and SIEGFRIED DIETRICH^{1,2} — ¹Max-Planck-Institut für Intelligente Systeme, Heisenbergstr. 3, 70569 Stuttgart — ²IV. Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

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]. Recent experiments have demonstrated a fluctuation-induced lateral trapping of spherical colloidal particles immersed in a binary liquid mixture near its critical demixing point and exposed to chemically patterned substrates [2].

Inspired by these experiments, we study the critical Casimir effect for elongated colloids of cylindrical shape. When the colloidal particles are close to a chemically structured substrate, a critical Casimir torque acting on the colloids emerges. Our analysis indicates that critical Casimir interactions are capable to achieve well-defined, reversible alignments both of chemically homogeneous and of Janus cylinders [3].

[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)

[3] M. Labbé-Laurent, M. Tröndle, L. Harnau, S. Dietrich, preprint;

arXiv:1311.3814 (2013)

CPP 40.3 Thu 11:45 ZEU 260

Fundamental measure approaches to liquid crystals — ●RENÉ WITTMANN, MATTHIEU MARECHAL, and KLAUS MECKE — Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany

Fluids of hard spherocylinders exhibit a rich phase behavior including isotropic, nematic and smectic-A phases. A density functional for anisotropic hard bodies can be constructed in terms of tensorial weighted densities (FMT) which depend on geometry and position of only one single oriented particle [1]. Within a new geometric method to derive the exact low-density functional we introduce a mixed measure of two bodies which can be expanded to the original tensor series. We compare this fundamental mixed measure theory (FMMT) to approximated results and Monte-Carlo simulations.

Closed formulas for the Frank elastic coefficients and the restriction to parallel spherocylinders verify the consistency of FMMT analytically. The isotropic - nematic interfacial tension remarkably improves on earlier, only qualitatively correct predictions [2]. For the first time we obtain a phase diagram of hard spherocylinders which can be quantitatively compared to simulations. We find a first order nematic to smectic-A transition up to an aspect ratio of at least 40. The increased computational effort and the relevance of other components of the functional is discussed.

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

[2] R. Wittmann and K. Mecke, *J. Chem. Phys.*, submitted (2013).

CPP 40.4 Thu 12:00 ZEU 260

New Monte Carlo method to simulate interfacial free energies — ●FABIAN SCHMITZ, PETER VIRNAU, and KURT BINDER — Institut für Physik, Johannes Gutenberg-Universität Mainz, Deutschland

We present a new Monte Carlo simulation method to calculate the interfacial tension γ between two phases, e.g. liquid-gas-coexistence or crystal-liquid coexistence. The knowledge of the precise value of the interfacial tension is of vital importance for the understanding of nucleation phenomena and the prediction of nucleation rates.

The method is based on a thermodynamic integration. In the initial state, the two homogeneous phases are within two completely separate boxes with periodic boundary conditions in all directions. In the final state, the two phases coexist in a joint box and thereby form two interfaces. The free energy difference ΔF between the initial and the final state is then given by the surface free energy of the two interfaces. The method is applicable to Ising (lattice gas) models as well as colloidal systems with Lennard-Jones or hard sphere potentials. Since

a finite interface has additional entropic terms depending on the box dimensions, a systematic analysis of the finite size effects is carried out.

CPP 40.5 Thu 12:15 ZEU 260

Cluster Formation in Systems of Magnetic Cubes at Low Temperatures. — ●JOE G. DONALDSON¹ and SOFIA KANTOROVICH^{1,2} — ¹Faculty of Physics, University of Vienna, Boltzmannngasse 5, A-1090 Vienna, Austria — ²Ural Federal University, Lenin av. 51, Ekaterinburg, 620083, Russia.

Colloidal synthesis has progressed to the point where a large array of particle geometries is now readily accessible. For example, recently realised systems of cubic particles now form an active area of research [Meijer et. al, *Soft Matter*, 2013]. The non-spherical shape of these particles provides a perfect scenario in which to study the consequences of external anisotropy on cluster formation. In addition, an internal anisotropy can be present for particles formed of magnetic compounds. In this work we describe and account for the structures formed in a magnetic cubic colloidal system at low temperatures. Our system is comprised of monodisperse cubes with centrally positioned point magnetic dipoles. Two separate scenarios are considered: one where the dipole orientation is along the [100] crystallographic direction, and the other, along [111]. We present analytical energy calculations in quasi two dimensions of the possible structures formed at 0K. The approach taken here is an extension of that employed for spheres by

[Propkópieva et. al, *Phys. Rev. E*, 2009]. These predictions are compared to replica exchange molecular dynamics computer simulations at low temperatures. The findings of this work are later hoped to aid in the determination of thermodynamic properties of these colloids at room temperature.

CPP 40.6 Thu 12:30 ZEU 260

Dynamic States in Driven Liquid Crystals of Hard-Spherocylinders — ●ELLEN FISCHERMEIER, MATTHIEU MARECHAL, and KLAUS MECKE — Institut für Theoretische Physik, FAU Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen, Germany

We investigate a system of hard spherocylinders, arguably the simplest model system for rodlike colloidal liquid crystals, under the influence of an external periodic potential with Langevin dynamics simulation. The chosen potential acts solely on the orientation of each individual particle and represents a preferred direction of alignment which rotates in the x-y-plane. Depending on the rotation frequency of the external potential and the packing fraction of the particles we discover a variety of nonequilibrium states which can be compared to results of density functional theory [1].

We also report on the possibility of coupling this simulation to a Lattice Boltzmann framework to include long range hydrodynamic interactions.

[1] A. Härtel et al., *Phys. Rev. E* 81, 051703 (2010)

CPP 41: Nanoparticles and Composite Materials

Time: Thursday 9:30–13:15

Location: ZEU 222

CPP 41.1 Thu 9:30 ZEU 222

Ultra-fast in-situ SAXS/WAXS on the nucleation and growth of CdS quantum dots — ●ANDREAS SCHIENER and ANDREAS MAGERL — Lehrstuhl für Kristallografie und Strukturphysik, Staudtstraße 3, 91058 Erlangen

Quantum dots provide due to their unique electrical and optical properties a high potential for applications in solar cells, photo diodes, as medical tracers, and in numerous other fields. Although many synthesis routes for the controlled fabrication are known and well established, a fundamental understanding of the nucleation and growth process is still missing. In this contribution we present a combined ultra-fast in-situ SAXS and WAXS study, which gives for the first time a direct experimental insight into the evolution of the crystalline and morphological structure of CdS quantum dots in the up to now unexplored time regime between 0.1 ms and 2.5 ms with a time resolution of down to 0.01 ms. The precipitation reaction of CdS takes place along a continuous free liquid jet, which converts the time scale into a length scale to address these short reaction times. A prominent cluster structure with the diameter of about 1 nm was observed both in the SAXS and in the WAXS signal. The formation mechanism of the final quantum dots is dominated by oriented attachment of these primary clusters.

CPP 41.2 Thu 9:45 ZEU 222

Simulation of disorder effects in the optical spectra of homogeneously alloyed CdSeS nanocrystals — ●DANIEL MOURAD¹, TANGI AUBERT², ANTOINE GUILLE², EDOUARD BRAINIS², and ZEGER HENS² — ¹Institut für Theoretische Physik, Universität Bremen — ²Physics and Chemistry of Nanostructures, Ghent University

Monodisperse, homogeneously alloyed CdSe(x)S($1-x$) nanocrystals, which can be grown by means of colloidal synthesis, allow for a gradual tailoring of the absorption/emission properties by variation of the composition. Besides the nonlinear variation of the excitation gap as a function of x ("bowing"), the optical spectra also show an additional alloy-only feature on the S-rich side. The homogeneity of the alloying could be confirmed by Raman spectroscopy [Aubert et al., *Chem. Mater.* 25(12), 2388 (2013)].

Starting from a tight-binding model for the constituents CdSe and CdS, we try to understand the electronic and optical properties of this quantum dot ensemble system in theory. In our approach alloy effects are simulated exact in the disorder, i.e. the single-particle energies and wave functions are calculated for a large ($N \approx 50$) number of nanocrystals in a stochastic approach for each concentration x . Then, dipole and Coulomb matrix elements are calculated for each realization in order to obtain the light-matter coupling and the many-body properties

of this system within the configuration interaction method [Mourad and Czycholl, *Eur. Phys. J. B* 78, 497 (2010)]. It is shown that alloying relaxes the selection rules that apply to pure CdSe and CdS and the relation between simulation and experimental results is discussed.

CPP 41.3 Thu 10:00 ZEU 222

Templating Carbon Nanotubes with Block Copolymer Micelles — ●MATTHIAS M. L. ARRAS, CHRISTOPH SCHILLAI, and KLAUS D. JANDT — Chair of Materials Science (CMS), Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Löbdergraben 32, 07743 Jena, Germany

Control over carbon nanotube dispersion and spatial arrangement are the major issues of carbon nanotube/polymer composites.

In the present study we present the use of an amphiphilic block copolymer as a dispersing agent and its spherical micelles as a template at the same time.

High molecular weight polystyrene-block-poly(2-vinylpyridine) micelles are formed in a selective solvent and ultrasonicated together with unfunctionalized multi-walled carbon nanotubes(MWCNTs). Transmission electron microscopy pictures reveal that the MWCNTs segregate to the interface of the block copolymer.

The obtained structures depend on the length of the MWCNTs and range from split ring to wrapping of multiple micelles. The segregation to the interface is explained by a relieved chain stretching in the block copolymer interface upon crowding with MWCNTs.

We propose application as conducting polymer composites with very low percolation threshold or as a metamaterial.

CPP 41.4 Thu 10:15 ZEU 222

Harnessing thermoplasmonics for actuation of hydrogel — ●HANG ZHANG, MARTIN MÖLLER, and AHMED MOURRAN — DWI - Leibniz Institut für Interaktive Materialien, Aachen, Germany

Significant attention has been drawn in the last decades on the localized surface plasmon resonance (LSPR) of noble metal nanoparticles featuring remarkable photothermal energy conversion. In this regard, we report on a near-infrared driven hydrogel actuation system consisting of gold nanorods (AuNRs) embedded in Poly(N-isopropylacrylamide) (PNIPAM) network. Illuminations instantly heat the AuNRs and transform the hydrogel from the swollen state to the state above the lower critical solution temperature, causing the polymer network and the water to segregate. As a result, the expansion or contraction of the hydrogel can be remotely modulated, which is reversible, fast and local. The report discusses the possibility for actuation (amplitude, frequency) and the significance of the irradiation time and frequency on the hydrogel response dynamics.

CPP 41.5 Thu 10:30 ZEU 222

Tracer Diffusion Studies of Tailored Nanostructured Composites — ●ANDY KIESSLING¹, VINCENT LE HOUÉROU², CHRISTIAN GAUTHIER², and ECKHARD BARTSCH¹ — ¹Department of Physical Chemistry, Albertstr. 21, 79104 Freiburg, Germany — ²Institut Charles Sadron - CNRS UPR 022, 23 rue du Loess - BP 84047, 67034 Strasbourg cedex 2, France

Volatile organic compounds in solvent cast film formation act as softener and leave behind films of high material strength after evaporation. Water-based systems lack this ability, but this drawback can be circumvented by the combination of components with complementary properties like high T_g core - low T_g shell polymer dispersions. The improved properties of coatings from water-based core-shell polymer dispersions like enhanced scratch resistance are attributed to a layer of restricted mobility of the polymer surrounding the high T_g cores. Studies addressing the molecular origin of the observed macroscopic enhancements are scarce. Applying a tracer diffusion method (Forced Rayleigh Scattering) allows an analysis of the nanostructured composites on a molecular level on different length scales. Through the superposition of two laser beams, a holographic grating is created. The diffusion of the dye is detectable as time decay of an optical Bragg scattering signal. Interpretation and modeling of the signal provide information about the mobility of the tracer in various film compartments, which is characterized by diffusion coefficients and diffusion lengths. These investigations are complemented by studies on the macroscopic film properties, notably the behavior when submitted to sliding contact.

CPP 41.6 Thu 10:45 ZEU 222

Temperature Dependent Luminescence and Dephasing of Gold Nanorods — ●ALEXANDER KONRAD¹, FRANK WACKENHUT¹, MARTIN HUSSELS¹, ALFRED J. MEIXNER¹, and MARC BRECHT^{1,2} — ¹Universität Tübingen, IPTC, 72076 Tübingen, Germany — ²Zürcher Hochschule für Angewandte Wissenschaften, IAMP, 8401 Winterthur, Switzerland

The one-photon luminescence of noble metal nanoparticles is a well known phenomenon, but its underlying physics is not yet completely understood. The reason for the common use of nanoparticles in optics is lying in their ability to exhibit plasmons, which are responsible for a large scattering cross section of nanoparticles and probably also partly for their photoluminescence. Quantifying plasmons is possible spectroscopically by their resonance frequency and dephasing time, depending on intrinsic and extrinsic properties. We present measurements of the one-photon luminescence emitted by single gold nanorods (GNR) to propose its causally underlying processes. Therefore, we determined the resonance frequency and dephasing times of single GNRs as a function of temperature from ambient down to cryogenic temperatures (295K-1.6K) and assumed the plasmon as a Lorentzian oscillator. The determined increase of the dephasing times with decreasing temperature follows a simple Debye-model for electrons and phonons in bulk materials confirming the plasmonic origin of the one-photon luminescence. The temperature independent contributions for dephasing are assigned mainly to the processes: electron-electron-scattering, electron-surface-scattering and radiative damping.

CPP 41.7 Thu 11:00 ZEU 222

A drug delivery system based on calcium carbonate sub-micron particles — BOGDAN PARAKHONSKIY^{1,2}, ●ALBRECHT HAASE³, YULIA SVENSKAYA^{1,4}, and RENZO ANTOLINI¹ — ¹BIOtech center, Dept. of Industrial Engineering, University of Trento, Mattarello (TN), Italy — ²A.V. Shubnikov Institute of Crystallography Russian Academy of Science, Moscow, Russia — ³Department of Physics, University of Trento, Povo (TN), Italy — ⁴Saratov State University, Saratov, Russia

We present synthesis, loading, and release of sub-micron carriers in form of polycrystalline vaterite. The experimental characterization of the system shows excellent suitability for drug delivery applications, like perfect biocompatibility, high substance loading, and multiple controllable payload release mechanisms. We present in detail two of these mechanisms, one is a fast pH-dependent release due to a rapid degradation of the carriers in buffers below pH 7. The second is a delayed burst release due to a crystal phase transition from vaterite to calcite, predestined for scheduled admission. The release dynamics of both processes can be further controlled by the molecular properties of the payload, variation of carrier size, or additional layers. First in vitro experiments show high cellular uptake efficiency of the vaterite carriers.

ers. Possible applications in photodynamic therapy of cancer in the gastrointestinal tract will be discussed.

15 min break

CPP 41.8 Thu 11:30 ZEU 222

Morphological and swelling behavior of Block Copolymer/Nanoparticles Composites — ●CHRISTIAN LEWIN, LARISA TSARKOVA, and ALEXANDER BÖKER — DWI at the RWTH Aachen, Forckenbeckstraße 50, 52074 Aachen, Germany

Among polymer-inorganic composites, block copolymers loaded with metal particles attract particular research interest due to their technological potential in nanoelectronics, nanolithography and sensing applications. We study the influence of selectively deposited gold nanoparticles (Au-NPs) on the micro-phase separation behavior and on macroscopic swelling of block copolymer films. We report solvent vapor annealing of Polystyrene-block-poly(2-vinylpyridine)/gold nanoparticles composites with varying concentration of loaded Au-NPs that have been subjected to solvent vapor annealing under controlled temperature and partial vapor pressure of the solvent vapor. Measurements of the swollen film thickness with in-situ ellipsometry revealed that the NPs concentration has a clear effect on the solvent up-take, as well as on the phase behavior of composite films. In particular we observed an unusual type of surface patterning which was attributed to fine tuning of interfacial interactions by NPs. Performing swelling experiments using controlled annealing set up is essentially important for generating reproducible and therefore comparable data on the behavior of composite films in confined geometry and hence for providing novel insights into the understanding of complex nanoheterogeneous systems.

CPP 41.9 Thu 11:45 ZEU 222

Anomaly in thermal and mechanical properties of SBR/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 Faiencerie, L-1511, Luxembourg

Filling elastomers with nanoparticles generally leads to changes in the relaxation behavior of the matrix molecules. Using dynamic mechanical analysis (DMA) and temperature modulated calorimetry (TMDSC), we investigated the influence of different amounts of untreated, hydrophilic alumina nanoparticles on the properties of a model rubber system (SBR). Beside a reinforcement effect seen in the complex elastic moduli, small amounts of nanoparticles of about 2 wt% interestingly lead to an acceleration of the relaxation modes responsible for the thermal glass transition. This leads to a minimum in the glass transition temperature as a function of nanoparticle content in the vicinity of this critical concentration. The frequency dependent elastic moduli are used to discuss the possible reduction of the entanglement of rubber molecules as one cause for this unexpected behavior.

CPP 41.10 Thu 12:00 ZEU 222

Resolving the inner structure of nanoparticles by means of solvent contrast variation with SAXS — ●RAUL GARCIA-DIEZ, CHRISTIAN GOLLWITZER, and MICHAEL KRUMREY — Physikalisches Technische Bundesanstalt, Berlin, Germany

Synthetic latex prepared by multiple-addition emulsion polymerisation present a spherical core-shell structure which can be revealed by Small Angle X-ray Scattering (SAXS) and resolved in conjunction with solvent contrast variation. This method allows the traceable characterization of the size and size distribution of the particles in suspension as well as an insight in its radial structure and an electron density determination, using both the Guinier and Fourier region of the scattering curves along an extended *q*-range.¹ A novel approach to contrast variation based on the anomalous scattering effect of the solvent close to an X-ray absorption edge is presented and compared to the more classical case of latex suspensions in sucrose solutions.

¹ N.Dingenouts, J.Bolze, D.Potschke, M.Ballauff; *Analysis of polymer latexes by small angle x-ray scattering*, Advances in Polymer Science Vol. 144, pp 1-47 (1999)

CPP 41.11 Thu 12:15 ZEU 222

Using the Interplay of Different Techniques to Understand the Microscopic Origin of the Macroscopic Material Behavior — ●GERALD SCHNEIDER, THOMAS GLOMANN, JÜRGEN ALLGAIER, and

DIETER RICHTER — Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science and Institute for Complex Systems, Germany

Intense research has led to substantial progress towards understanding polymer melts and nanocomposites. For that purpose, knowledge of the single chain dynamics is of particular interest. It is important for modeling or predicting the macroscopic material response needed for the target oriented engineering of new hybrid materials starting from the single molecule. It may lead to optimized materials ranging from the classical car tire to battery or fuel cell applications.

In polymer melts, different microscopic processes, such as diffusion, reptation, contour length fluctuations, etc. add up to the total response at the macroscopic length-scale. Additionally, in composites with inorganic nanoparticles hard impenetrable walls impose constraints on polymer melts, by limiting the accessible regions. Such a confinement significantly affects the polymer dynamics when the interparticle distances and the dimensions of the embedding polymer chains are comparable.

The talk illuminates the relationship between the microscopic dynamics and the macroscopic application, exploiting different experimental techniques, such as dielectric spectroscopy, rheology, neutron scattering and spectroscopy.

CPP 41.12 Thu 12:30 ZEU 222

Method for quantitative and qualitative detection of nano-sized particles emitted from paper and packaging materials

— ●VOLKER UHL¹, RICARDO VIZCAYA¹, and ANDREAS KORNHERR² —
¹Austrian Research Institute for Chemistry and Technology (OFI), Vienna, Austria — ²Mondi Uncoated Fine & Kraft Paper GmbH, Austria

Paper is a complex material which consists of an organic fiber matrix with embedded inorganic filler particles and various different additives. Such a compound material tends to the emission of various fiber fragments, filler particles, and additive residues when being exposed to mechanical stress. We present the acoustic dust tester - a new method to qualitatively and quantitatively determine particulate matter emis-

sions in the nanosized range from paper surfaces: In a measuring chamber the paper is exposed to a well defined mechanical stress induced via acoustic waves. The exit air from the chamber is led to aerosol characterizing and sampling instruments, e.g. a condensation particle counter and an electro-mobility spectrometer. We present the concentration and particle size distribution of emitted nanoparticles from a number of different paper and packaging materials determined via this method. The detection of nanoparticles is of increasing importance both because a very low level of paper dusting is a quality characteristic for high grade papers and also to ensure that any possible health risks arising from small respirable dust particles due to the handling of paper can be completely excluded.

Invited Talk

CPP 41.13 Thu 12:45 ZEU 222

Growth kinetics of metal nanoparticles on polymer surfaces

— ●EZZELDIN METWALLI — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Dispersed metal nanoparticles (nps) in a polymer matrix are essential for many technological applications, including biological imaging, thin film technology, magnetic recording media, optoelectronics and sensors. Real time investigation of the evolution of nps size and shape during the in-situ metal deposition on polymer thin films enables a fine tune of magnetic and electric properties. Metals in their atomic state are deposited on several homopolymer and block copolymer films by DC magnetron system [1]. With the unprecedented time resolution of 10 milliseconds, the growth kinetics of the metal nps on the polymer surfaces is monitored using in-situ GISAXS. An exponential growth of nps size on all polymer surfaces is observed. Below a certain critical nps size, an initial fast particle growth is due to high particle mobility. A slower kinetics at concentrated metal dispersion is due to the strong metal-metal interactions. The metal growth kinetics study for many chemically different homopolymer films explains the long-time debated high selectivity characteristics of metals towards one block in block copolymer based nano-templates. 1- E. Metwalli et al. Langmuir 29, 6331 (2013)

CPP 42: Friction and Lubrication

Time: Thursday 9:30–11:30

Location: ZEU 114

CPP 42.1 Thu 9:30 ZEU 114

High Resolution Force Measurements of Host-Guest Complex Interaction

— ●BIANCA BOZNA¹, JOHANNA BLASS^{1,2}, MARCEL ALBRECHT³, GERHARD WENZ³, and ROLAND BENNEWITZ^{1,2} —
¹INM - Leibniz Institute for New Materials, Saarbrücken, Germany — ²Physics Department, Saarland University, Saarbrücken, Germany — ³Organic Macromolecular Chemistry, Saarbrücken, Germany

Surfaces with well-defined friction and adhesion properties such as high shearing but low peeling resistance are required for many of technical applications. We currently develop a novel surface material based on cyclodextrin assemblies with switchable friction and adhesion characteristics mediated by ditopic guest molecules. As a mandatory step towards achieving this aim, we investigate the friction forces between two surfaces functionalized with β -cyclodextrin in two different configurations. The friction measurements were performed on β -cyclodextrin modified gold surfaces in both pure water and ditopic guest solution (adamantane). The gold surface was functionalized with β -CD molecules whose thiol end groups provide a covalent bond to the substrate. The level of coverage by CD molecules on the gold surface was tested by cyclic voltammetry. Using high resolution friction force measurements we prove that the friction force between the two opposing β -cyclodextrin layers strongly increases in ditopic guest solution when compared to pure water. The long term goal of this research is to develop switchable adherent surfaces that can find applications in biotechnology or medical devices.

CPP 42.2 Thu 9:45 ZEU 114

Structural arrangement of hyaluronan and DPPC bilayer under high hydrostatic pressure

— ●THOMAS ZANDER¹, FLORIAN WIELAND¹, MIN WANG², AKANKSHA RAJ², VASYL HARAMUS¹, ANDRA DEDINAITE², PER CLAEISSON², and REGINE WILLUMEIT¹ —
¹Helmholz-Zentrum Geesthacht, Institute of Materials Research, D-21502 Geesthacht — ²KTH Royal Technical Institute, Department of Chemistry, SE-100 44 Stockholm

Articular joints are bio-lubrication systems with the lowest friction coefficients found in nature. The friction coefficient is provided by the synovial fluid, which is an intricate composition of different macromolecules (e.g. phospholipids and hyaluronan) and which keeps the exceptional good lubrication properties even under high loads and shear rates. It is thought that the different constituents form complex structures in order to enable this low friction coefficients.

In order to gain information about the structure of the hyaluronan-phospholipid bilayer samples we performed X-Ray reflectivity measurements at different hydrostatic pressures (1bar - 2kbar). The obtained data clearly reveal the adsorption of hyaluronan to the phospholipid bilayer. Interestingly the structure of the hyaluronan-DPPC layer varies as the molecular weight of hyaluronan is changed. This is supported by DLS and surface-pressure isotherms which show also a stronger interaction with a decreasing molecular weight of hyaluronan.

CPP 42.3 Thu 10:00 ZEU 114

Determining the friction coefficient of a nanometer sized colloid by molecular dynamics simulations

— ●ZORAN MILIČEVIĆ¹, DAVID M. SMITH^{2,3}, and ANA-SUNČANA SMITH^{1,3} — ¹Institut für Theoretische Physik, FAU Erlangen-Nürnberg, Erlangen, Germany — ²Computer Chemie Centrum, FAU Erlangen-Nürnberg, Erlangen, Germany — ³Institute Rudjer Bošković, Zagreb, Croatia

Estimation of the transport coefficients of colloids in liquids is still a challenging task for computer simulations. Apart from technical difficulties, the limits of the validity of the Stokes-Einstein relation have not yet been fully established. Here, we calculate the diffusion and the friction coefficients of a nanometer sized particle in water by performing extensive molecular dynamics simulations using the GROMACS software package. We first provide a protocol for defining the hydrodynamic radius of the particle. We then show that both the diffusion and the friction coefficient, and hence the water shear viscosity, can be calculated independently. This is used to demonstrate the validity of the Stokes-Einstein relation in this regime. We compare the obtained results to the shear viscosity calculated independently from pure wa-

ter simulations and the Green-Kubo relation. We investigate various approaches and present an analysis of simulation conditions required for accurate predictions of transport coefficients, with a particular emphasis on the mass and the size of the spherical particle, as well as the size of the system. As an interesting extension, we study the transport properties of a particle in water subject to a constant electric field, which breaks the otherwise isotropic nature of the system.

CPP 42.4 Thu 10:15 ZEU 114

Switchable friction using asymmetric contacts of stimulus-responsive and non-responsive polymer brushes — ●SISSI DE BEER^{1,2}, EDIT KUTNYANSZKY¹, and JULIUS VANCOS¹ — ¹Materials Science and Technology of Polymers, University of Twente, Enschede, the Netherlands — ²Jülich Supercomputing Centre, Forschungszentrum Jülich, Jülich, Germany

Stimulus responsive (SR), solvated polymers can switch between an expanded and a collapsed conformation via external stimuli. Using molecular dynamics simulations and atomic force microscopy experiments, we show that such SR polymers can be employed to control the frictional response of two opposing polymer brushes in relative sliding motion. By using a brush composed of SR polymers in contact with a non-responsive polymer brush, the overlap between the opposing brushes can be switched ON/OFF: When both brushes are swollen, polymers of the opposing brushes interdigitate, which results in high friction upon shearing. In contrast, when the SR brush is collapsed, the solvent maximizes the interaction with the non-responsive brush. The latter circumvents both brushes from interdigitating, which results in low friction upon shearing.

Invited Talk

CPP 42.5 Thu 10:30 ZEU 114

Tribology of colloidal systems — ●CLEMENS BECHINGER — Universität Stuttgart, 2. Physikalisches Institut, Stuttgart — Max-Planck-Institut für Intelligente Systeme, Stuttgart

Friction between solids is responsible for many phenomena like earthquakes, wear or crack propagation. Unlike macroscopic objects which only touch locally due to their surface roughness, spatially extended contacts form between atomically flat surfaces. They are described by the Frenkel-Kontorova (FK) model where a monolayer of interacting particles on a periodic substrate potential is considered. In addition to the well-known slip-stick motion the FK-model also predicts the forma-

tion of kinks and antikinks which largely reduce the friction between the monolayer and the substrate. Here, we report the direct observation of kinks and antikinks in a two-dimensional charge-stabilized colloidal crystal which is driven across different types of ordered substrates created by interfering laser beams. We show that the tribological properties only depend on the number and density of such excitations which propagate through the monolayer along the direction of the applied force.

- T. Bohlein, J. Mikhael, and C. Bechinger, Observation of kinks and antikinks in colloidal monolayers driven across ordered surfaces, *Nature Materials* 11, 126 (2012).

- T. Bohlein, and C. Bechinger, Experimental observation of directional locking and dynamical ordering of colloidal monolayers driven across quasiperiodic surfaces, *Phys. Rev. Lett.* 109, 058301 (2012).

Invited Talk

CPP 42.6 Thu 11:00 ZEU 114

Contact and Friction of Rough Adhesive Surfaces — ●MARK ROBBINS¹, LARS PASTEWKA^{1,2}, and TRISTAN SHARP¹ — ¹Johns Hopkins University, Baltimore, Maryland, USA — ²Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg, Germany

Experimental surfaces typically have roughness on a wide range of length scales. This roughness greatly reduces the fraction of the area that is in intimate molecular contact and thus can contribute to friction and adhesion. The talk will first describe recent numerical calculations of elastic contact between rough surfaces with nominally flat or spherical geometries on large scales. An efficient Greens function approach allows calculations for systems with roughness on nanometer to micrometer scales to be performed with atomic resolution in the contact. Results for a wide range of geometries can be collapsed using simple scaling relations that depend on the root mean squared surface slope, sphere radius, elastic modulus, and work of adhesion. The scaling relations explain why adhesive interactions have little effect unless the surfaces are extremely smooth or soft. The traditional Fuller-Tabor model for adhesion of rough surfaces is shown to be qualitatively inconsistent with the simulations. The effect of atomic scale plasticity on contact and adhesion is surprisingly small. The talk will conclude by considering how forces in the contact area give rise to friction. Friction shows strong scale effects and the partial slip assumed in many contact models is not found in contacts with dimensions of nanometers to micrometers.

CPP 43: Glasses and Glass Transition (joint session with DY/DF) I

Time: Thursday 11:45–12:45

Location: ZEU 114

Invited Talk

CPP 43.1 Thu 11:45 ZEU 114

Dynamics and thermodynamics of glassy polymers below the glass transition temperature — ●DANIELE CANGIALOSI — Paseo M Lardizabal 5, 20080 San Sebastian, Spain

Glass-forming systems constitute an important class of materials. Among different aspects, the dramatic slowing down of the dynamics when decreasing temperature and the possible connection between such slowing down and the thermodynamics of the glass-former have been intensively studied. It has been speculated that mere extrapolation of the dynamics and thermodynamics to temperatures below the glass transition temperature (T_g) produces a singularity at a finite temperature, with divergent relaxation time and vanishing configurational entropy. Here the dynamics and thermodynamics are studied at temperatures as low as $T_g - 40$ K by performing enthalpy recovery experiments on glassy polymers for times up to 10^7 - 10^8 seconds. We find a single stage recovery behavior for temperatures larger than about $T_g - 10$ K. A double stage recovery is observed for $T < T_g - 10$ K. The enthalpy recovered after the two-stage decay equals that extrapolated from the melt, whereas partial enthalpy recovery occurs in the first decay. From the analysis of the time to reach each equilibrium it is found that the equilibration time corresponding to the first stage recovery exhibits relatively low activation energy, whereas the second one exhibits activation energy similar to that of the polymer segmental relaxation. These results indicate a complex scenario of the dynamics and thermodynamics below T_g with multiple equilibration steps and leave open the question the finite temperature singularity.

CPP 43.2 Thu 12:15 ZEU 114

Excess heat capacity and fictive temperature of polystyrene

in a wide range of cooling and heating rates — ●GUNNAR SCHULZ¹, TIMUR VASILIEVICH TROPIN², YEONG ZEN CHUA¹, JÜRN W. P. SCHMELZER¹, and CHRISTOPH SCHICK¹ — ¹Institut für Physik, AG Polymerphysik, Universität Rostock, Rostock, Germany — ²Frank Laboratory of Neutron Physics, Joint Institut for Nuclear Research, Dubna, Moscow region, Russia

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

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

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

CPP 43.3 Thu 12:30 ZEU 114

Glassy dynamics and physical aging in fucose saccharides as studied by Infrared- and Broadband Dielectric Spectroscopy — ●WILHELM KOSSACK¹, KAROLINA ADJRANOWICZ², MAGDALENA TARNACKA¹, WYCLIFFE KIPROP KIPNUSU¹, MATEUSZ DULSKI², EMANUEL URANDU MAPESA¹, KAMIL KAMINSKI², SEBASTIAN PAWLUS², MARIAN PALUCH², and FRIEDRICH KREMER¹ — ¹Universität Leipzig,

Linnestr.5, Molekülphysik, 04103 Leipzig, Germany — ²Institute of Physics, University of Silesia, ul. Uniwersytecka 4, 40-007 Katowice, Poland

Fourier Transform InfraRed (FTIR) and Broadband Dielectric Spectroscopy (BDS) are combined to study both, the intra- and intermolecular dynamics for two isomers of glass forming fucose, far below and above the calorimetric glass transition temperature, T_g . It is shown, that the various IR-active vibrations exhibit in their spectral

position and oscillator strength quite different temperature dependencies, proving their specific signature in the course of densification and glass formation. The coupling between intra- and inter-molecular dynamics is exemplified by distinct changes of IR active ring vibrations far above the calorimetric glass transition temperature at about $1.16T_g$, where the dynamic glass transition (α relaxation) and the secondary β relaxation merge. — For samples physically annealed below T_G slower isothermal relaxation times than extrapolated from liquid state are observed.

CPP 44: Charged Soft Matter I

Time: Thursday 9:30–12:30

Location: ZEU 118

CPP 44.1 Thu 9:30 ZEU 118

Absorption of a charged polymer star by an oppositely charged polyelectrolyte brush — ●MAJID FARZIN^{1,2}, TORSTEN KREER¹, and JENS-UWE SOMMER^{1,2} — ¹Leibniz institute for polymer research dresden — ²Technical University of Dresden

By means of molecular dynamics simulations, we investigate the interactions between a polyelectrolyte brush and an oppositely charged polymer star. We explicitly include counterions and vary the strength of Coulomb interactions in two fashions; by varying the Bjerrum length of fully charged polymers and by changing the charge fraction of grafted chains for the Bjerrum length close to that of water. The simulations show that there is a critical Bjerrum length below which the polymer star is located outside the brush. For larger values of the Bjerrum length, the polymer star is absorbed by the brush. In the case of charge fraction variation, the polymer star is absorbed by the brush at all charge fractions. Also, we observe that, in the vicinity of the critical Bjerrum length or for small charge fractions, the shape of the polymer star is pancake-like.

CPP 44.2 Thu 9:45 ZEU 118

Inhomogeneous swelling of Polyelectrolyte Multilayers in water — ●MAXIMILIAN ZERBALL¹, RALF KÖHLER², and REGINE VON KLITZING¹ — ¹Institut für Chemie - Stranski-Laboratorium, Technische Universität Berlin, Str. 17.Juni 124, 10623 Berlin — ²Institut für Weiche Materie und funktionelle Materialien, Helmholtz-Zentrum Berlin, Hahn - Meitner-Platz 1, 14109 Berlin

Polyelectrolyte Multilayer (PEM) are organic films built up via subsequent adsorption of oppositely charged polyions. They are interesting materials for nanofabrication and fundamental science due to the possible and precise tunability of their physico-chemical properties, as thickness roughness, or adsorption of molecules and particles. PEM are highly sensitive to external parameter like the relative humidity (RH) of the ambient atmosphere. Increase of RH causes water uptake and swelling, accompanied with changes of the permeability for water. In order to use these films as sensors or for optical devices it is important to understand and to control the swelling mechanism. Neutron Reflectometry (NR) is an excellent tool to investigate the inner structure of PEMs. The usage of PEMs consisting of two different blocks, a deuterated block and a protonated block creates an additional surface inside the PEM which is detectable for NR and allows detecting an inner and an outer part of the sample, but with chemically identical composition. The results show an inhomogeneous swelling across the PEM.

CPP 44.3 Thu 10:00 ZEU 118

Adsorption Behavior of Catanionic Surfactant Mixtures at the Air-Water Interface and in Freestanding Foam Films — ●HEIKO FAUSER, MARTIN UHLIG, and REGINE VON KLITZING — Technische Universität Berlin, Stranski-Laboratorium Institut für Chemie, Straße des 17. Juni 124, 10623 Berlin

Although the application of liquid foams is widespread, too little is yet understood about their stability control. One way to tune liquid foam films is the use of oppositely charged surfactant mixtures. Due to electrostatic attraction highly surface active aggregates are formed. Our study addresses the question of whether the adsorption of equimolar or irregular catanionic complexes and thus a variation in surface composition governs foam film properties.

Mixtures of the anionic surfactant SDS with the cationic C12TAB are investigated. We compare the adsorption behavior at liquid/air interfaces and in freestanding foam films at different total concentrations

and varying mixing ratio.

Surface tension measurements reveal a high surface activity for these mixtures already at very low concentrations. The same high surface activity is detected over a broad regime varying the mixing ratio. In contrast Thin Film Pressure Balance measurements reveal a variation in the foam film properties. Foam film thickness and stability varies with the mixing ratio. We also discuss a strong impact on adsorption kinetics and foaming of these mixtures.

This shows that for different catanionic surfactant mixtures surface composition and foam film properties changes.

CPP 44.4 Thu 10:15 ZEU 118

Structure of electrolyte solutions in complex solvents — ●MARKUS BIER — Max Planck Institute IS und University of Stuttgart, Germany

Since recently quite some theoretical as well as experimental effort is devoted to investigate structural properties of electrolyte solutions in which the solvent cannot be considered as a structureless medium. The most prominent example are solvents formed by binary liquid mixtures whose components interact differently with the ions. Consequently the presence of ions can influence the phase diagram of the solvent, e.g. the location of the miscibility gap. Conversely, a solvent mixture close to its critical demixing point can perturb the structure of the ions. This contribution discusses the changes of the structure of electrolyte solutions in binary liquid mixture solvents as one approaches the critical demixing point [1,2]. It is explained how the partial pair distribution functions evolve upon approaching the critical point of the mixture from a monotonic decay on the length scale of the Debye length via an oscillatory decay, reached by Kirkwood crossovers, towards a monotonic decay on the length scale of the bulk correlation length. This scenario is a key to understand recent experimental findings related to the structure of electrolyte solutions in complex solvents.

References:

- [1] M. Bier, A. Gambassi and S. Dietrich, *J. Chem. Phys.* **137**, 034504 (2012).
- [2] M. Bier and L. Harnau, *Z. Phys. Chem.* **226**, 807 (2012).

CPP 44.5 Thu 10:30 ZEU 118

Impedance spectroscopy of ions at liquid-liquid interfaces — ●ANDREAS REINDL and MARKUS BIER — Max Planck Institute IS und University of Stuttgart, Germany

One possibility to examine interfaces between two immiscible liquids is by means of impedance spectroscopy. In order to interpret the measured impedance spectra, frequently equivalent (electric) circuits where each element is intended to represent a certain microscopic process are fitted to the data. In this contribution we highlight two major problems with this procedure and propose a novel approach to avoid them. Both problems of the commonly used one-step fitting of impedance data are related to the phenomenon of actually obtaining circuit elements which lump bulk and interfacial properties together. This leads to the first, more technical problem of a possible overfitting of the bulk elements at the expense of an underfitting of the interfacial elements, which compromises the accuracy of the desired interfacial quantities. The second, more fundamental problem is related to the assignment of microscopic processes to circuit elements, which we show to be approximative in general and which requires ad-hoc interpretations for one-step fitting. In order to overcome both difficulties, we propose to disentangle bulk and interfacial circuit elements by means of a two-step fitting procedure, which we demonstrate for theoretically determined impedance data and which can be expected to be used similarly for real data.

Reference:

A. Reindl and M. Bier, Phys. Rev. E. **88**, 052312 (2013).

CPP 44.6 Thu 10:45 ZEU 118

Effective Interactions in Protein-Salt Solutions Approaching Liquid-Liquid Phase Separation — ●MARCELL WOLF¹, FELIX ROESEN-RUNGE¹, FAJUN ZHANG¹, ROLAND ROTH², and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik, Auf der Morgenstelle 10, Universität Tübingen, 72076 Tübingen, Germany — ²Institut für Theoretische Physik, Auf der Morgenstelle 14, Universität Tübingen, 72076 Tübingen, Germany

We present an experimental study combined with a theoretical discussion of the effective interactions in protein solutions approaching a liquid-liquid phase separation (LLPS) induced by addition of multivalent metal ions [1,2]. The reduced second virial coefficient, B_2/B_2^{HS} , is used to describe the interaction and discussed with theoretical predictions for colloidal systems. We have determined the salt and protein partitioning in the two coexisting phases, which provides the isothermal binodal of the LLPS in the (c_p, c_s) plane. Two sets of samples, away from and at the LLPS binodal were measured by static light scattering (SLS) and small angle X-ray scattering (SAXS) to determine the second virial coefficient. In all cases, B_2/B_2^{HS} is negative in the condensed regime, and increases upon approaching the upper critical point in the (c_p, c_s) plane. The results are compared with a simple colloidal model with isotropic short-ranged attraction and a thermodynamic criterion based on the reduced second virial coefficient. We discuss the application of this theoretical prediction to interpret experimental observations. [1] M. Wolf et al., J. Mol. Liq., submitted; [2] F.Zhang et al., Soft matter 8, 2012, 1313.

15 min. break

CPP 44.7 Thu 11:15 ZEU 118

Response of the Water Hydration Layer around a Spherical Solute to an Electric Field — ●CHRISTIAN SCHAAF and STEPHAN GEKLE — Biofluid Simulation and Modeling, Universität Bayreuth

The behavior of charged particles in aqueous solutions is strongly influenced by the hydration layer. Near these particles the dielectric response function ϵ is an anisotropic and space-dependent tensor in contrast to the scalar quantity it is in bulk water.

Using molecular dynamics (GROMACS) and linear response theory we calculate the radial component of the local dielectric response tensor in water around a spherical solute. We find an oscillatory behavior for the radial component of the response function which we explain by the nonlocal permittivity calculated from bulk properties. These calculations show that on small length scales the response is mostly determined by the field geometry of a point charge and much less by the actual solute-water interface.

Understanding the dielectric response is essential for the behavior of ion distributions and may improve the accuracy of implicit solvent simulations.

CPP 44.8 Thu 11:30 ZEU 118

Specific Ion Binding to Amphiprotic Surface Groups and the pH Dependence of the Hofmeister Series — ●NADINE SCHWIERZ¹ and ROLAND R. NETZ² — ¹Physik Department, Technische Universität München, Germany — ²Physik Department, Freie Universität Berlin, Germany

Ion binding to amphiprotic surface groups is one of the central mechanisms for ion-specificity if ionizable groups are present on the surface of a macromolecule. To gain insight into the microscopic mechanism, we use a combination of atomistic simulations and Poisson-Boltzmann theory and bridge from computational results to macroscopic experimentally accessible properties.

In our modeling approach, we first extract single-ion surface interaction potentials at atomistically resolved surfaces composed of uncharged carboxyl-groups and of charged carboxylate-groups. The surface affinity of single ions depends strongly on whether the carboxyl group is dissociated or not and is even reversed for cations.

Phase diagrams, based on long-ranged forces between two heterogeneous surfaces containing carboxyl and carboxylate groups interacting across electrolyte solutions, feature direct, reversed and altered Hofmeister series in dependence of the salt concentration and pH. The results provide a microscopic explanation for the pH dependence of the Hofmeister series due to specific and diverse ion binding to carboxyl and carboxylate surface groups.

CPP 44.9 Thu 11:45 ZEU 118

Elastic/viscoelastic properties of polyelectrolyte multilayer films (PLL/HA) as measured by AFM nano-indentation — ●JOHANNES HELLWIG and REGINE VON KLITZING — Stranski-Laboratorium, Department of Chemistry, TU Berlin, Strasse des 17. Juni 124, D-10623 Berlin

In recent years smart biomaterials have become a highly developing field of interest for biomedical applications, e.g. drug delivery(1). The layer-by-layer (LbL) technique (2) 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 elastic(3) and viscoelastic properties of LbL coated poly(L-lysine)/hyaluronic acid PLL/HA films were studied by colloidal probe atomic force microscopy. It was shown that the indentation modulus of PLL/HA films measured in different pH and ionic strength of the surrounding medium changes. Increasing the temperature shows a slight decrease in modulus at higher temperatures. Furthermore the viscoelastic film behaviour was measured and calculated by stress relaxation and creep compliance measurements.

CPP 44.10 Thu 12:00 ZEU 118

Observation of Polarization in the Leaning Plane of a Bent-Core Molecular Compound — ●NATTAPORN CHATTHAM^{1,2}, MARIA GABRIELA TAMBA¹, EDUARD WESTPHAL⁴, HIDEO TAKEZOE^{1,3}, RALF STANNARIUS¹, CARSTEN TSCHIERKE⁴, and ALEXEY EREMIN¹ — ¹Otto-von-Guericke-Universität Magdeburg, IEP/ANP, D-39106 Magdeburg, Germany — ²Department of Physics, Faculty of Science, Kasetsart University, Bangkok 10900 Thailand — ³Department of Organic and Polymeric Materials, Tokyo Institute of Technology, Tokyo 152-8552, Japan — ⁴Institute of Chemistry, Martin-Luther-University Halle-Wittenberg, D-06120 Halle, Germany

Bent-core molecules have been of interest to liquid crystal scientists for over decades. Designing molecules and identifying their phase structures provide much knowledge to understand the complexity of molecular organization of these phase structures. In the conventional polar SmCP (B2) phase of bent-core mesogens, the tilting of molecules with respect to the layer normal occurs by the rotation about the bend direction, so that the spontaneous polarization is perpendicular to the tilt plane. In contrast, molecules lean within their bend plane in the SmC leaning phase, where the polarization is in the leaning plane and deviates from the layer plane. Here we report a clear evidence of this structure, i.e., the polarization lying in the leaning plane from direct observations of thick freely suspended films at inclined incidence under an in-plane electric field. The induced polarization was also confirmed by second-harmonic generation (SHG) activity. This work was supported by Alexander von Humboldt Foundation.

CPP 44.11 Thu 12:15 ZEU 118

Modelling of neutron spectroscopy of hydrogen bonded organic crystals using first principles density functional theory — ●SANGHAMITRA MUKHOPADHYAY — ISIS Facility, Rutherford Appleton Laboratory - STFC, Harwell Science and Innovation Campus, Didcot, Oxfordshire, OX11 0QX

Hydrogen bonded organic crystals are important both for fundamental chemical interests as well as for technological applications. Neutron spectroscopy is used to understand these hydrogen bonded materials experimentally. The static lattice dynamics are not often suitable to analyse these spectroscopic results, specially, where complex picosecond order dynamics are involved. In this work we will present our work on modelling of neutron spectroscopic results using first principles lattice and molecular dynamics.

We employed state-of-the-art calculations based on plane wave pseudo potential density functional theory to predict the structure of croconic acid, an organic molecular crystal, showed room temperature ferroelectricity, and compared with in-house neutron diffraction and inelastic neutron scattering (INS) spectrum to understand the nature of hydrogen bonds in this material. The quasielastic spectrum were calculated by analysing the trajectory of the molecular dynamical simulations and also compared with experiments.

We will discuss the neutron spectrum in terms of motions of hydrogen ions. The calculated Born effective charge tensors are used to understand the nature of dynamic charges and the origin of ferroelectricity.

CPP 45: The Collapsed State of Polymers: From Physical Concepts to Applications and Biological Systems (symposium, CPP/DY/BP)

Time: Thursday 9:30–12:15

Location: HSZ 02

Invited Talk CPP 45.1 Thu 9:30 HSZ 02

Why do polymer collapse and polymer topology frustrate each other — ●ALEXANDER Y. GROSBERG — Department of Physics and Center for Soft Matter Research, New York University, NY, USA

Polymer topology is most commonly studied in the context of a melt or concentrated solution. Here, the role of topological constraints is discussed in the context of a single chain swelling or collapse behavior, both in kinetics and in equilibrium (the latter in case topology is quenched, one way or another). Biological aspects are discussed in the context of both chromatin and proteins.

Invited Talk CPP 45.2 Thu 10:00 HSZ 02

Nanoscopy of nuclear Genome Structure — ●CHRISTOPH CREMER — Institute of Molecular Biology (IMB), D-55128 Mainz — Kirchhoff-Institute of Physics (KIP) University Heidelberg, D-69120 Heidelberg — Institute of Pharmacy and Molecular Biotechnology (IPMB) University Heidelberg, D-69120 Heidelberg

Numerical models as well biochemical data indicate a decisive functional role of genome nanostructure; but due to the conventional resolution limits of far-field light microscopy, direct light microscopic tests of such models were believed to be impossible. However, novel developments in optical technology and photophysics succeeded to radically overcome these conventional limits. With such "superresolution" techniques, it has become possible to analyze nuclear genome structure with a greatly enhanced light optical resolution down to a few tens of nanometer. Application examples will be presented on the use of such "nanoscopy" procedures to measure in cell nuclei the size of individual small chromatin domains, of replication and transcription complexes, as well as the spatial distribution of individual nuclear proteins and of short specifically labelled DNA sequences. It is anticipated that the wealth of nanoscale information on nuclear genome nanostructure accessible by the novel superresolution approaches will substantially contribute to the theoretical understanding of the folding in space and time of the huge polymers called chromosomes, and its functional consequences.

Invited Talk CPP 45.3 Thu 10:30 HSZ 02

Blood Clotting Inspired Polymer Physics — ●ALFREDO ALEXANDER-KATZ — Massachusetts Institute of Technology

Nature has devised creative and efficient ways of solving complex problems, and one of these problems is that of blood clotting in flowing conditions. In fact, nature has used a novel combination of polymer physics and chemistry that enhances the self-healing propensity of a vessel when strong flows are present while avoiding coagulation when the flow is diminished, a rather counter-intuitive phenomenon. Underlying this process is a globular biopolymer, the so-called von Willebrand Factor, whose function is strongly regulated by flow. In this talk I will present our work on this macromolecule starting from the single molecule approach and building up to the multi component system that more closely resembles blood. I will emphasize how new

concepts have emerged from trying to understand such a complex system, in particular I will show how these polymers can display giant non-monotonic response to shear, as well as a very large propensity to form polymer-colloid composites in flow while being a stable dispersed suspension in quiescent conditions. In fact, the aggregation behavior is universal and can be explained with simple scaling arguments. These novel concepts and results are in principle not unique to blood clotting and can have important ramifications in other areas.

15 min. break

Invited Talk CPP 45.4 Thu 11:15 HSZ 02

Modeling dynamic spatial genome organization in yeast — ●CHRISTOPHE ZIMMER — Institut Pasteur, 25 rue du Docteur Roux, 75015 Paris

The spatial organization and dynamics of chromosomes plays important roles for gene expression, DNA repair and replication, but its underlying principles remain poorly known. We will present quantitative experimental data and simulation results showing that the territorial organization the interphase yeast nucleus and the dynamics of chromosomes can be largely predicted by a model based on generic polymer physics with a minimal set of DNA sequence-specific constraints and assumptions. We will also discuss extensions of our budding yeast model to other organisms and address implications of this model for a quantitative understanding of DNA repair.

Invited Talk CPP 45.5 Thu 11:45 HSZ 02

Ring polymers in the melt state: the physics of crumpling — ●RALF EVERAERS¹ and ANGELO ROSA² — ¹Laboratoire de Physique et Centre Blaise Pascal, ENS Lyon, CNRS UMR5672, 46 allée d'Italie, 69364 Lyon, France — ²SISSA - Scuola Internazionale Superiore di Studi Avanzati, Via Bonomea 265, 34136 Trieste (Italy)

The conformational statistics of ring polymers in melts or dense solutions is strongly affected by their quenched microscopic topological state. The effect is particularly strong for non-concatenated unknotted rings, which are known to crumple and segregate and which have been implicated as models for the generic behavior of interphase chromosomes. Here we use a computationally efficient multi-scale approach to identify the subtle physics underlying their behavior, where we combine massive Molecular Dynamics simulations on the fiber level with Monte Carlo simulations of a wide range of lattice models for the large scale structure. We show that (i) topological constraints may be neglected on scales below the standard entanglement length, L_e , (ii) that rings with a size $1 \leq L_r/L_e \leq 30$ exhibit nearly ideal lattice animal behavior characterized by primitive paths which are randomly branched on the entanglement scale, (iii) that larger rings are weakly swollen relative to ideal lattice animals with gyration radii $\langle R_g^2(L_r) \rangle \propto L_r^{2\nu}$ and $\nu \approx 1/d > 1/4$, and (iv) that ring melts can be *quantitatively* mapped to coarse-grained melts of *interacting* randomly branched primitive paths.

CPP 46: Focus Session: Slow Dynamics in Glasses and Granular Matter I (original: DY, joined by CPP)

The transition into an amorphous solid state is typically accompanied by the observation of slow dynamics. The understanding of such transitions from first principles has seen progress in many of its aspects recently, including nonlinear response, residual stresses, and non-affine deformations. The Focus Session provides an overview of common phenomena and of general concepts in the physical picture of disordered materials. (Organizers M. Sperrl and A. Zippelius)

Time: Thursday 9:30–12:30

Location: HÜL 186

Invited Talk CPP 46.1 Thu 9:30 HÜL 186

The memory of sand — ●MATTHIEU WYART — New York University
Complex systems are characterized by an abundance of meta-stable states. To describe such systems statistically, one must understand how states are sampled, a difficult task in general when thermal equilibrium does not apply. This problem arises in various fields of science, and here I will focus on a simple example, sand. Sand can flow until one jammed configuration (among the exponentially many possible ones) is reached. I will argue that these dynamically-accessible configurations are atypical, implying that in its solid phase sand "remembers" that it was flowing just before it jammed. As a consequence, it is stable, but barely so. I will argue that this marginal stability answers long-standing questions both on the solids and liquid phase of granular materials, and will discuss tentatively the applicability of this idea to other systems.

Invited Talk CPP 46.2 Thu 10:00 HÜL 186

Complex rheology at the jamming transition: shear thickening, shear thinning, shear banding — ●CLAUS HEUSSINGER — Institut für theoretische Physik, Universität Göttingen

The jamming paradigm aims at providing a unified view for the elastic and rheological properties of materials as different as foams, emulsions, suspensions or granular media. The usefulness of such a unifying concept hinges on the presence or absence of phenomena that are in some sense *universal*.

In this contribution, we discuss how certain features in the particle interactions affect the rheological properties of the material. First, we discuss the effect of frictional forces, and show how the jamming phase diagram has to be modified as compared to the frictionless scenario [1,2]. Essential findings are a discontinuous and hysteretic jamming transition, as well as a shear thickening regime where frictionless particles are generically shear thinning.

Secondly, we investigate the role of attractive interactions between the particles [3]. For weakly attractive systems a fragile solid develops which displays self-organization towards a minimal (isostatic) connectivity. Moreover, the measured flow curves have unstable regimes, which lead to persistent shearbanding. These features are rationalized by establishing a link between rheology and inter-particle connectivity, which also provides a minimal theoretical model to describe the flow curves.

[1] CH, PRE (2013). [2] M. Grob. CH, A. Zippelius, arXiv (2013). [3] E. Irani, P. Chaudhuri, CH, arXiv (2013).

CPP 46.3 Thu 10:30 HÜL 186

Stress-birefringence information in three-dimensional binary granular packings — ●PEIDONG YU, STEFAN FRANK-RICHTER, and MATTHIAS SPERL — Institut für Material Physik im Weltraum, Köln, Deutschland

We report our newly developed 3D stress-birefringence technique and its application in a binary static packing. We show how we precisely determine the stress state of one single spherical particle from its stress-birefringent response to external contacts. Such particles of two different sizes are used in a dense packing with different packing fractions. Based on the knowledge of one-particle calibration, we are able to define a transition point from the integrated stress-birefringent signal of the whole packing under changing packing fraction. Variations of these transition points with different size ratio and specie number ratio of the two particle species are measured and discussed.

CPP 46.4 Thu 10:45 HÜL 186

Jamming of Frictional Particles: a First Order Phase Transition — ●MATTHIAS GROB¹, CLAUS HEUSSINGER², and ANNETTE ZIPPELIUS^{1,2} — ¹Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Deutschland — ²Institut für Theoretische Physik,

Universität Göttingen, Göttingen, Deutschland

With numerical simulations, we produce flow curves for dense frictional granular media with features different from the frictionless analog. When the strain rate is controlled and increased, a smooth transition from inertial to plastic flow is observed below a critical volume fraction. Above this packing fraction, the transition becomes discontinuous as a hallmark of friction. Upon an increase of packing fraction, the flow curves show hysteretic behaviour, the emergence of a yield stress and the divergence of the shear viscosity - each at a different packing fraction. All the reported behaviour is reproduced with a simple model for a non-equilibrium first order phase transition. An inherent feature of dense frictional granular rheology is that the transition from flowing to jammed states is reentrant with transient jam-and-flow states in between which are, within the models' framework, metastable flow states.

15 min. break

CPP 46.5 Thu 11:15 HÜL 186

Vibrational Masking of Critical Decay in the Early beta-Relaxation Regime of Incoherent Intermediate Scattering Functions in Simulated Glass Forming Ni_{0.5}Zr_{0.5} — ●HELMAR TEICHLER — Institut f. Materialphysik, Univ. Göttingen

Results are presented concerning the origin of discrepancy between mode coupling theory (MCT) prediction for critical decay in the early beta-regime and molecular dynamics (MD) simulation data. The discrepancy is known since long in the literature and is heuristically ascribed to effects of atomic vibrations not fully taken into account in MCT. A proper theoretical treatment is missing so far. Here I present a formally exact framework for analyzing the MD data, which allows deducing the origin of the discrepancy and its quantitative description, and I apply it to MD simulated glass forming Ni_{0.5}Zr_{0.5}. The approach relates incoherent intermediate scattering functions (ISFs) from atomic trajectories, which show the discrepancy, to those from inherent structure (IS), which are in agreement with MCT. Cumulant expansion of the ISFs demonstrates that the discrepancy reflects the vibrational density of states, with minor effect of the Boson peak. The results for Ni_{0.5}Zr_{0.5} rely on the fact that there are only weak correlations between atomic vibrations and IS relaxation displacements in the beta-regime, and that the essential part of the vibrational displacements distribution acts Gaussian-like.

CPP 46.6 Thu 11:30 HÜL 186

Glass Transition of Yukawa Systems: Crossover from Hard Sphere to Soft Sphere Limits — ●ANOOSHEH YAZDI¹, ALEXEI IVLEV², SERGEI KHRAPAK², ADAM WYSOCKI³, HARTMUT LÖWEN⁴, and MATTHIAS SPERL¹ — ¹Institut für Materialphysik im Weltraum, Deutsches Zentrum fuer Luft- und Raumfahrt, 51147 Köln, Germany — ²Max-Planck-Institut für extraterrestrische Physik, 85741 Garching, Germany — ³Institute for Advanced Simulation and Institute of Complex Systems, Forschungszentrum Jülich, 52425 Jülich, Germany — ⁴Institut für Theoretische Physik II, Heinrich-Heine-Universität Düsseldorf, 85741 Düsseldorf, Germany

The mode-coupling theory for ideal glass transitions (MCT) is applied to the single and double Yukawa potential systems. Glass transition curves are obtained in the full range of two control parameters: the screening parameter κ , which is the inverse screening length, and the interparticle potential strength Γ . With increasing κ along the transition, glass form factors and effective packing fractions undergo a crossover from the one-component plasma (OCP) limit, which resembles a very soft sphere system, to a hard sphere system (HSS). The entire transition diagram can be described by analytical functions. Surprisingly and different from those of other potentials, glass transition curves are found to be shifted but otherwise identical to the

melting curves in the control parameter plane.

CPP 46.7 Thu 11:45 HÜL 186
rheology near jamming—the influence of lubrication forces —
 ●MOUMITA MAITI and CLAUS HEUSSINGER — Georg-August University
 of Goettingen, Goettingen, Germany

The talk discusses the role of different dissipation forces on the rheological properties of highly dense non-Brownian suspensions. The focus is on the random close packing limit ("jamming") where particle motion is limited due to steric volume exclusion. We define a simplified lubrication force where we change the dissipation mechanisms by tuning the range of the interaction. Two densities are considered, one is near jamming the other further away. For both densities, a crossover is seen from 'inertia' dominated flow to viscous flow by changing the lubrication range. Interestingly, we observe that velocity fluctuations are independent of the different dissipation mechanisms ("universal") near jamming. Away from jamming this universality is lost and an unexpected non-monotonic dependence is seen. We present an understanding of our findings in terms of geometric constraints of random-close packing and a decoupling of dissipative forces and particle trajectories.

CPP 46.8 Thu 12:00 HÜL 186
Lattice Boltzmann Simulations for Glass-Forming Liquids —
 ●SIMON PAPANIKOLAOU^{1,2} and THOMAS VOIGTMANN^{1,2} — ¹Institut für
 Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt,
 Köln, Germany — ²Zukunftskolleg und Fachbereich Physik,
 Universität Konstanz, Germany

In continuum mechanics, the Navier-Stokes (NS) equation is used to study fluid flows. The Lattice Boltzmann (LB) model is an efficient method to find solutions of the NS equation of Newtonian liquids even

for complex flow geometries.

Complex fluids, such as glass formers, colloidal suspensions, or granular media, display a wide range of non-Newtonian flow effects, determined by the interplay between slow structural dynamics on the microscopic scale, and the mesoscopic flow field. Prominent examples are shear thinning and yield stresses, leading to plug flow in channels.

Starting from first principles, mode coupling theory of the glass transition is able to provide constitutive equations that describe the history effects determining the flow of glass-forming fluids. We present results from a new LB scheme that allows to include memory-integral effects in fluid-mechanics simulations.

CPP 46.9 Thu 12:15 HÜL 186
Slow convection in densely packed granular mixtures —
 ●FRANK RIETZ and RALF STANNARIUS — University of Magdeburg,
 Institute of Experimental Physics, Department of Nonlinear Phenomena

Handling of granulate in partly filled rotating containers is a common situation in industrial processes. Contrary to ensembles of loosely packed grains, the container can be filled so dense that fluidization is limited to a shallow surface layer. Then, the deeper layers are in a locked state, only creeping motions on longer time scales are possible.

We study such a situation in a flat rotating container of aspect ratio 1 that is almost completely filled with a bidisperse mixture. Irrespective of the limited mobility of the grains we observe nonuniform segregation patterns accompanied by slow convective motion. Many features of the convection flow amplitude, like regular oscillatory modulations of the convection velocity, cessations and spontaneous reversals of the circulation are comparable to convection in ordinary liquids at high Rayleigh numbers, in geometries with aspect ratio 1.

[1] F. Rietz & R. Stannarius, Phys. Rev. Lett. 108, 118001 (2012).

CPP 47: Focused Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale VI (original: O, joined by CPP)

Time: Thursday 10:30–13:15

Location: TRE Ma

Topical Talk **CPP 47.1 Thu 10:30 TRE Ma**
Localization at the edge of 2D topological insulator by Kondo impurities — ●BORIS ALTSHULER¹, IGOR ALEINER¹, and VLADIMIR YUDSON² — ¹Physics Department, Columbia University, New York, NY 10027, USA — ²Institute for Spectroscopy, Russian Academy of Sciences, Troitsk, Moscow 142190, Russia

Recent interest to the topological insulators [1] is inspired by the fact that their boundaries host gapless electronic excitations, which are extended and make the system conductive even in the presence of a potential disorder. 1D edge of a 2D topological insulator is predicted to have perfect conductance ($2e^2/h$): right and left moving electrons carry opposite spins and potential disorder cannot flip spins and thus causes neither back-scattering nor the usual 1D localization.

What if there are localized spins coupled to the edge electrons? It turns out that the conductivity is still perfect provided that this coupling conserves the z-projection of the total spin of the impurities and electrons. Magnetic anisotropy violates this conservation and causes the backscattering even at $T=0$, i.e. an arbitrary small density of the spins with arbitrary weak anisotropy of the coupling leads to Anderson localization of the edge states in long enough samples [3]. The conclusion follows from the mapping of the electron-spin coupling to the well-studied problem [2] of disordered Luttinger liquid.

1. M.Z. Hasan and C.L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
2. T. Giamarchi and H.J. Schulz, Phys. Rev. B 37, 325 (1988).
3. B.L. Altshuler, I.L. Aleiner, V.I. Yudson Phys. Rev. Lett 111, 086401 (2013)

CPP 47.2 Thu 11:00 TRE Ma
Multiple Exciton Generation in Si and Ge Nanoparticles with high pressure core structures — ●STEFAN WIPPERMANN¹, MARTON VÖRÖS², DARIO ROCCA³, ADAM GALI⁴, GERGELY ZIMANYI², and GIULIA GALLI² — ¹Max-Planck-Institute for Iron Research, Düsseldorf — ²University of California, Davis — ³Universite de Lorraine, Nancy — ⁴Budapest University of Technology and Economics

Multiple exciton generation (MEG) in semiconductor nanoparticles (NPs) is a promising path towards surpassing the Shockley-Queisser limit in solar energy conversion efficiency. Recent studies demonstrate

MEG to be more efficient in NPs than in the bulk, including Si. However, the increased efficiency is observed only on a relative energy scale in units of the gap: quantum confinement (QC) effects believed to be responsible for efficient MEG in NPs, also increase their optical gap, swiftly shifting the MEG threshold beyond the solar spectrum.

We present density functional and many body perturbation theory calculations of the electronic, optical, and impact ionization properties of Si and Ge nanoparticles (NPs) with core structures based on high-pressure bulk Si and Ge phases. Si and Ge particles with a BC8 or ST12 core structure exhibit significantly lower optical gaps and multiple exciton generation (MEG) thresholds, and an order of magnitude higher MEG rate than diamondlike ones of the same size (1).

(1) S. Wippermann et al., Phys. Rev. Lett. 110, 046804 (2013)

CPP 47.3 Thu 11:15 TRE Ma
Advanced time-evolution method for optical absorption spectra calculations — ●TOBIAS SANDER and GEORG KRESSE — Computational Materials Physics, University of Vienna, Sensengasse 8/12, 1090 Vienna, Austria

The Green's function formalism from many-body perturbation theory gives access to electronic structure calculation within the quasiparticle picture, as well as provides for calculating optical absorption spectra. Within the traditional ansatz [1], a Bethe-Salpeter like equation for the polarizability is solved. This requires to diagonalize an in general non-hermitian and complex matrix (BSE matrix). Usually, the off-diagonal elements of the BSE matrix are neglected and this is referred to as Tamm-Dancoff approximation. The computational effort can be reduced by using the time-evolution ansatz [2] which avoids the matrix diagonalization. We present a method based on the time-evolution algorithm, that finally avoids storing and diagonalizing the BSE matrix. This leads to a reduction of the scaling w.r.t the system size N from N^5 to N^3 . Finally, we present first results for typical systems.

[1] S. Albrecht, L. Reining, R. Del Sole, G. Onida, PRL 80, 4510 (1998)

[2] W. G. Schmidt, S. Glutsch, P. H. Hahn, F. Bechstedt, PRB 67, 085307 (2003)

CPP 47.4 Thu 11:30 TRE Ma
New starting point for the calculation of optical properties — ●IGOR RESHETNYAK^{1,2} and LUCIA REINING^{1,2} — ¹Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DSM, F-91128 Palaiseau, France — ²European Theoretical Spectroscopy Facility (ETSF)

The Bethe-Salpeter Equation based on Hedin's GW approximation to the self-energy is a powerful approach for describing electron-hole interactions in optical properties and photo-absorption spectra. However, in its current formulation it is both computationally heavy and displays cancellation effects not accounted for analytically. We discuss the sources of these cancellations and the possibility of putting them forward explicitly. We furthermore assess alternative formulations and sets of approximations to the BSE. For each of them we examine its behavior on model systems as well as their computational applicability. Finally we suggest possible directions for further investigations.

CPP 47.5 Thu 11:45 TRE Ma
Electron-Energy Loss and Inelastic X-ray Scattering of CuO from First Principles — ●CLAUDIA RÖDL, FRANCESCO SOTTILE, MATTEO GATTI, and LUCIA REINING — Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DSM, 91128 Palaiseau cedex, France and European Theoretical Spectroscopy Facility (ETSF)

Even though the strongly correlated transition-metal oxide CuO has many fields of application (potential absorber material in photovoltaic devices, pigment in glass and ceramics, building block of cuprate superconductors,...), surprisingly little is known about its electronic excitations from a theoretical point of view. The band gap and all electronic excitations in its vicinity are governed by the intricate interplay between itinerant $O\ 2p$ and localized $Cu\ 3d$ electrons. Complex many-body effects, that are still not well understood nowadays, determine the screening of the electron-electron interaction.

Electron-energy loss and inelastic x-ray scattering experiments yield direct access to the wave-vector- and frequency-dependent loss function $-\text{Im}\ \varepsilon_{\mathbf{G}\mathbf{G}'}^{-1}(\mathbf{q}, \omega)$, and, hence, to the screened Coulomb interaction W . We use time-dependent density-functional theory (TDDFT) to calculate the loss spectrum of CuO and discuss the occurring d - d and plasmon excitations. This allows us, by comparing theory and experiment, to assess the quality of the screened Coulomb interaction which is a key quantity for many-body approaches, for instance, GW and Bethe-Salpeter calculations.

CPP 47.6 Thu 12:00 TRE Ma
Optical Spectra from Molecules to Solids: Insight from Many-Body Perturbation Theory — ●CATERINA COCCHI and CLAUDIA DRAXL — Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany

The spurious long-range behavior of time-dependent (TD) density functional theory (DFT) is a well known source of error in describing bound excitons in solids. Remarkably, TD-DFT is often able to capture the optical features of isolated systems, even with the most simple exchange-correlation kernels, like the TD local density approximation. With the example of molecular crystals, we aim at solving the puzzle when and why TD-DFT can be relied on. We answer this question by confronting TD-DFT with many-body perturbation theory (GW and Bethe-Salpeter equation), which is the most accurate methodology to describe optical excitations in solids. Our results are obtained with the all-electron code "exciting" (<http://exciting-code.org>), where all the quantities entering the two formalisms are treated on the same footing [1]. In-depth analysis allows us to identify the shortcomings of TD-DFT in predicting the excitonic spectra of extended systems and to understand when this methodology is capable of providing correct results.

[1] S. Sagmeister and C. Draxl, Phys. Chem. Chem. Phys. 11, 4451 (2009)

CPP 47.7 Thu 12:15 TRE Ma
Relativistic Solar Cells — ●PAOLO UMARI¹, EDOARDO MOSCONI², and FILIPPO DE ANGELIS² — ¹Dipartimento di Fisica e Astronomia, Università di Padova, via Marzolo 8, I-35131 Padova, Italy — ²Computational Laboratory for Hybrid/Organic Photovoltaics (CLHYO), CNR-ISTM, Via Elce di Sotto 8, I-06123, Perugia, Italy
 Hybrid AMX₃ perovskites (A=Cs, CH₃NH₃; M=Sn, Pb; X=halide) have revolutionized the scenario of emerging photovoltaic technologies. Indeed, a rapid evolution led, very recently, up to 15% efficient solar cells. CH₃NH₃PbI₃ has so far dominated the field, while the

similar CH₃NH₃SnI₃ has not been explored for photovoltaic applications, despite the reduced band-gap. Replacement of Pb by the more environment-friendly Sn would facilitate the large uptake of perovskite-based photovoltaics. Despite the extremely fast progress, the materials electronic properties which are key to the photovoltaic performance are relatively little understood. Here we develop an effective GW method incorporating spin-orbit coupling which allows us to accurately model the electronic, optical and transport properties of CH₃NH₃SnI₃ and CH₃NH₃PbI₃, opening the way to new materials design. The different CH₃NH₃SnI₃ and CH₃NH₃PbI₃ properties are discussed in light of their exploitation for solar cells, and found to be entirely due to relativistic effects.

CPP 47.8 Thu 12:30 TRE Ma
Solar nanocomposites with complementary charge extraction pathways for electrons and holes: Si embedded in ZnS — ●STEFAN WIPPERMANN¹, MARTON VÖRÖS², ADAM GALI³, FRANCOIS GYGI², GERGELY ZIMANYI², and GIULIA GALLI² — ¹Max-Planck-Institute for Iron Research, Düsseldorf — ²University of California, Davis — ³Budapest University of Technology and Economics

We propose that embedding silicon nanoparticles (NP) into amorphous, non-stoichiometric ZnS leads to promising nanocomposites for solar energy conversion. Using *ab initio* molecular dynamics simulations we show that upon high temperature amorphization of the host chalcogenide, sulfur atoms are drawn to the NP surface. We found that the sulfur content may be engineered to form a type II heterojunction, with complementary charge transport channels for electrons and holes, and that sulfur capping is beneficial to lower the nanoparticle gap, with respect to that of NPs embedded in oxide matrices. Our analysis was conducted using density functional theory with local and hybrid functionals and many body perturbation theory at the GW level.

CPP 47.9 Thu 12:45 TRE Ma
Ultraviolet photo-emission spectroscopies from Koopmans-compliant functionals — ●NGOC LINH NGUYEN¹, GIOVANNI BORGHI¹, ANDREA FERRETTI², ISMAILA DABO³, and NICOLA MARZARI¹ — ¹Theory and Simulations of Materials, École Polytechnique Fédérale de Lausanne, Station 12, 1015 Lausanne, Switzerland. — ²Centro S3, CNR-Istituto Nanoscienze, I-41125 Modena, Italy — ³Department of Materials Science and Engineering, The Pennsylvania State University, University Park, USA.

We study the photo-electron properties of organic photovoltaic molecules using Koopmans-compliant functionals [1] as well as the Perdew-Zunger self-interaction correction (PZ-SIC) [2] to density-functional theory. A simple method for simulating ultraviolet photo-emission spectra (UPS) of molecules has been implemented. It is based on a plane-wave approximation for the final states to account for the spectra intensities. Our calculations show that Koopmans-compliant functionals provide ionization potentials and electron affinities closely comparable with those obtained by many-body perturbation theory (GW). In addition, we find that UPS spectra computed imposing the Koopmans' condition on the PZ-SIC functional are in remarkable agreement with experimental results.

Refs: [1] I. Dabo, A. Ferretti, N. Poilvert, Y. Li, N. Marzari, and M. Cococcioni, Phys. Rev. B 82, 115121 (2010); [2] J. P. Perdew and A. Zunger, Phys. Rev. B 23, 5048 (1981).

CPP 47.10 Thu 13:00 TRE Ma
Self-consistent dynamical embedding in real space — ●WAEEL CHIBANI¹, XINGUO REN^{1,2}, PATRICK RINKE¹, and MATTHIAS SCHEFFLER¹ — ¹Fritz Haber Institute of the Max Planck Society, Berlin, Germany — ²Key Laboratory of Quantum Information, USTC, Hefei, China

Density-functional theory with its local-density (LDA) and generalized gradient approximations (GGA) is known to fail for localized states. To extend *ab initio* approaches to this domain, we have devised an embedding scheme that facilitates the treatment of the physically important part of a system with electronic structure methods, that are computationally too expensive for periodic systems, whereas the rest of the periodic system is treated with computationally less demanding approaches, i.e. LDA/GGA, in a self-consistent manner. Our scheme is based on the concept of dynamical mean-field theory (DMFT) [1]. However, in contrast to the original DMFT formulation for correlated model Hamiltonians, we consider here the unit cell as embedded cluster in an *ab initio* way, that includes all electronic degrees of freedom. The performance of our scheme is demonstrated by treating the embedded

region with hybrid functionals for simple bulk systems, e.g. Si or NiO. The total energy and the density of states converge rapidly with respect to the computational parameters and approach their bulk limit with increasing cluster size. By treating the embedded region with

GW we were able to improve the band gap using only a small cluster. The effect of self-consistency in *GW* for the embedded region will also be addressed. [1] A. Georges *et al.*, Rev. Mod. Phys. **68**,14 (2006)

CPP 48: The Collapsed State of Polymers: From Physical Concepts to Applications and Biological Systems (joint session with BP)

Time: Thursday 15:00–17:30

Location: ZEU 250

CPP 48.1 Thu 15:00 ZEU 250

Collapse and self-organization of polymer structures in poor solvent - A Monte Carlo Study — ●MARCO WERNER^{1,2}, CHRISTOPH JENTZSCH^{1,2}, and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden, Germany — ²Technische Universität Dresden, Germany

We investigate poor solvent effects in polymer structures such as single polymer globules [1], collapsed polymer brushes as well as self-assembled lipid bilayer membranes [2] by using the bond-fluctuation model with explicit solvent. Focussing on the coil-to-globule transition of single polymer chains we show that even in the case of very poor solvent our coarse grained lattice model avoids freezing effects and preserves dynamic fluctuations at the polymer-solvent interface in contrast to corresponding implicit solvent models. We demonstrate that fluctuations will be necessary for a complete description of the force-extension curve during the unravelling process of a single polymer globule. In particular in the region of coexistence of collapsed and stretched part we observe a fluctuating ensemble of globules along the chain, which smooths the force-extension curve.

[1] C. Jentzsch, M. Werner, und J.-U. Sommer, J. Chem. Phys. **138** (9), 094902 (2013).

[2] J.-U. Sommer, M. Werner, und V. A. Baulin, Europhys. Lett. **98**, 18003 (2012).

CPP 48.2 Thu 15:15 ZEU 250

Melts of unconcatenated and unknotted polymer rings revisited — ●JOACHIM WITTMER, HENDRIK MEYER, and ALBERT JOHNER — Institut Charles Sadron & CNRS, 23 Rue du Loess, 67034 Strasbourg CEDEX 2, France

A paradigmatic example for soft matter systems ruled by topological interactions is provided by melts of unconcatenated polymer rings. Recent computational studies suggest that sufficiently long rings become compact which begs the question of whether the irregular surfaces of these compact objects may be characterized by a finite fractal surface dimension $d_s < 3$. We revisit the scaling analysis of the intramolecular structure factor by Halverson *et al.* [J. Chem. Phys. **134**, 204904 (2011)] claiming $d_s \approx 2.8$. Our analysis suggests that this conclusion might be due to an inappropriate application of the Generalized Porod Law. We present then in the second part of our talk a “decorated Gaussian loop model” which does not require a finite fractal surface dimension $d_s < 3$. In this approach the topological interactions between different rings are taken into account by a self-similar and space-filling random tree of polydisperse Gaussian loops ranging from the entanglement length to a skeleton ring of length $N^{2/3}$. Individual rings are predicted to be marginally compact with an average chain size $R^2 \sim N^{2/3}(1 - 1/N^{1/3})$ where all prefactors have been omitted for clarity. Sluggish $1/N^{1/3}$ -corrections to the leading power-law behavior are also shown to arise for other experimentally relevant properties.

CPP 48.3 Thu 15:30 ZEU 250

Fractal globule as an artificial molecular machine — ●NECHAEV SERGEI — LPTMS (Orsay, France)

The relaxation of an elastic network, constructed by a contact map of a fractal (crumpled) polymer globule is investigated. We found that: i) the slowest mode of the network is separated from the rest of the spectrum by a wide gap, and ii) the network quickly relaxes to a low-dimensional (one-dimensional, in our demonstration) manifold spanned by slowest degrees of freedom with a large basin of attraction, and then slowly approaches the equilibrium not escaping this manifold. By these dynamic properties, the fractal globule elastic network is similar to real biological molecular machines, like myosin. We have demonstrated that unfolding of a fractal globule can be described as a cascade of equilibrium phase transitions in a hierarchical system. Un-

folding manifests itself in a sequential loss of stability of hierarchical levels with the temperature change.

CPP 48.4 Thu 15:45 ZEU 250

Conformation and Structural Changes of Diblock Copolymers with Octopus-Like Micelle Formation under the Influence of Water Vapor — ●KIRSTEN DAMMERTZ¹, MASOUD AMIRKHANI¹, CHRISTOPH JENTZSCH², JENS-UWE SOMMER^{2,3}, and OTHMAR MARTI¹ — ¹Institute of Experimental Physics, Ulm University — ²Leibniz-Institute of Polymer Research Dresden — ³Institute of Theoretical Physics, TU-Dresden

External stimuli like vapors, pressure or electric fields can be used to manipulate the polymer configurations of diblock-copolymers. Due to the conformational flexibility of such polymers, AB-diblock copolymers constitute a valuable tool to develop functional nanomaterials and devices.

We study the conformation and structural response of PS-*b*-PMMA, PS and PMMA adsorbed on mica under water vapor, respectively. At polymer concentrations below the minimum needed for the development of thin films, octopus-like surface micelles are formed. By applying water vapor to a system containing polar PMMA chains, additional mobility can be provided to the polymers. In contrast, PS is less affected since it does not contain a permanent dipole moment. Furthermore, collapse and decollapse effects were observed.

In addition to AFM measurements, we performed BFM Monte Carlo simulations to analyze the formation process of the micellar structures as well as their response to water vapor.

Invited Talk CPP 48.5 Thu 16:00 ZEU 250

Universal aspects of chromosome folding — ●ANGELO ROSA — Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste (Italy)

The dynamics of the mm-long chromatin (*i.e.*, DNA+histones) fibers in the cell nucleus is subject to strong topological constraints [Sikorav & Jannink (1994)]. In particular, their incomplete equilibration during interphase [Rosa & Everaers (2008)] results in territorial, crumpled globule-like chromosome conformations [Grosberg *et al.* (1993)].

It has been suggested [Rosa & Everaers, *ibid.*; Vettorel *et al.* (2009)], that this incomplete relaxation might underlie a subtle analogy between interphase chromosomes and corresponding solutions of non-concatenated ring polymers. Here, we start from our recent multi-scale computational approach for explicit construction of equilibrated solutions of giant ring polymers [Rosa & Everaers (2013); see talk by R. Everaers] to further explore the physical and biological consequences of this analogy.

We show that not only the territorial confinement [Cremer & Cremer (2001)] but also other characteristic features of chromosome folding such as their conformational statistics [Sachs *et al.* (1995); Lieberman-Aiden *et al.* (2009)] and the loop-on-loop structure of internal contacts [Cook (2010)] arise as a generic consequence of the polymeric nature of chromosomes. Integrated with biological information on intra- and inter-chromosomal interactions, our results pave the way for the systematic modeling of the nuclear structure and dynamics.

15 min break

CPP 48.6 Thu 16:45 ZEU 250

Effects of nucleosome positioning on condensation of short and long chromatin fibers — ROBERT SCHÖPFLIN¹, OLIVER MÜLLER¹, CHRISTIN WEINBERG¹, VLADIMIR B. TEIF², KARSTEN RIPPE², and ●GERO WEDEMANN¹ — ¹CC Bioinformatics, University of Applied Sciences Stralsund, Stralsund, Germany — ²Deutsches Krebsforschungszentrum & BioQuant, Heidelberg, Germany

In eukaryotes DNA is associated with proteins in a complex struc-

ture termed chromatin. The basic packaging unit of chromatin is the nucleosome in which DNA is wrapped around a histone octamer. Experiments indicate that chromatin has different packaging conditions connected to distinct activation states. Experimental evidence showed that packaging and activation states are closely linked to positions of nucleosomes on the DNA which are actively regulated. To improve the understanding of the interplay between nucleosome positions and chromatin structure we applied computer simulations of a coarse-grained chromatin model including fundamental physical properties such as elasticity, electrostatics and nucleosome interactions using a feedback-optimized replica exchange protocol. We calculated the effect of nucleosome positioning on the structure of polynucleosomes of different length scales, up to the size of a gene locus. We compared chromatin models based on synthetic positions with models based on experimentally derived nucleosome positions from cells at different stages of cell differentiation. Simulation results revealed a significant influence of nucleosome positions on the three dimensional structure of chromatin.

CPP 48.7 Thu 17:00 ZEU 250

Loop models in Magnetic Spin Ice crystals — ●LUDOVIC JAUBERT¹, MASUD HAQUE², and RODERICH MOESSNER² — ¹OIST, Okinawa, Japan — ²MPI-PkS, Dresden

Loops are ubiquitous in physics, either as tangible entities such as polymers, or as emergent phenomena, especially where we do not expect them. In this talk, we shall focus on the latter case, where loops appear as extended degrees of freedom in spin ice crystals.

Spin ice has become a canonical member of the large and growing family of frustrated magnets, where excitations take the form of magnetic monopoles. The ground state of this system is highly degenerate and can be mapped exactly onto a fully packed loop model. We studied the statistics of this model both in 2 and 3 dimensions [1], making contact with Stochastic-Loewner Evolution processes (SLE), percolation

and polymer physics, before illustrating implications of these results in related problems (Heisenberg magnets, itinerant electrons [2]).

[1] Jaubert, Haque, Moessner, PRL, 107, 177202 (2011)

[2] Jaubert, Pitaevski, Haque & Moessner, PRB, 85, 054425 (2012)

CPP 48.8 Thu 17:15 ZEU 250

Membrane-driven collapse of DNA macromolecules and semiflexible filamentous virus particles — ANASTASIA B. ARTEMIEVA¹, CHRISTOPH HEROLD², ANDREY G. CHERSTVY³, PETRA SCHWILLE¹, and ●EUGENE P. PETROV¹ — ¹Max Planck Institute of Biochemistry, 82152 Martinsried, Germany — ²BIOTEC, Technische Universität Dresden, 01307 Dresden, Germany — ³University of Potsdam, 14476 Potsdam-Golm, Germany

Interaction of (bio)macromolecules and colloidal particles with lipid membranes is one of the important problems of the modern bio-inspired soft matter physics. Earlier, we have found [1] that interaction of DNA molecules with strongly charged freestanding cationic lipid bilayers [2] leads membrane-mediated coil-globule transition of membrane-absorbed DNA macromolecules. Our recent experimental observations show that membrane-driven interactions at higher membrane charge densities are strong enough to induce the membrane-mediated collapse of much stiffer *fd* virus particles ($l_p \sim 2.2 \mu\text{m}$). We discuss these experimental findings in the framework of our new theoretical treatment [3] which takes into account membrane-polyelectrolyte electrostatic interactions, local membrane deformations, and polyelectrolyte bending rigidity.

[1] C. Herold, P. Schwille, and E. P. Petrov, *Phys. Rev. Lett.* **104** (2010) 148102.

[2] C. Herold, G. Chwastek, P. Schwille, and E. P. Petrov, *Langmuir* **28** (2012) 5518.

[3] A. G. Cherstvy and E. P. Petrov, *PCCP* (2014) in press.

CPP 49: Polymer Dynamics I

Time: Thursday 17:00–18:15

Location: ZEU 260

CPP 49.1 Thu 17:00 ZEU 260

Modeling high-molecular weight polymer melts: equilibration and rheological properties — ●LIVIA MOREIRA, GUOJIE ZHANG, TORSTEN STUEHN, KOSTAS DAOULAS, and KURT KREMER — Max Planck Institute for Polymer Research, Mainz

A modeling strategy is developed for studying rheological properties of high-molecular weight polymer melts described with microscopic detail. The microscopic model is generic but retains hard excluded volume interactions and realistic densities. Equilibrated configurations are generated by a backmapping strategy using a coarse-grained (CG) model representing polymer chains as strings of fluctuating blobs [1,2]. Each stands for one subchain of N_b microscopic beads. Varying N_b , a hierarchy of CG models with different resolutions is obtained. Within this hierarchy, CG configurations equilibrated at low-resolution are sequentially fine-grained into melts of higher resolution. Microscopic details are then introduced modifying the scheme of Auhl *et al* [3]. Backmapping involves only local polymer relaxation, thus the method is independent of chain length. This strategy is implemented to equilibrate melts with different persistence lengths and polymerization degrees up to 55 entanglement lengths, N_e . The N_e is quantified using primitive path analysis and effects of finite system-size and chain length are discussed. A master curve for the estimating N_e for different chain lengths and persistence lengths is provided. We comment on alternative estimations of N_e , e.g., from plateau modulus analysis. [1] Vettorel *et al*, *Soft Matter* (2010) 6, 2282 [2] Zhang *et al*, *Macromol. Chem. Phys.* (2013) 214, 214 [3] Auhl *et al*, *J. Chem. Phys.* (2003) 119, 12718

CPP 49.2 Thu 17:15 ZEU 260

Viscoelastic hydrodynamic interactions and anomalous CM diffusion in polymer melts — ●HENDRIK MEYER, A.N. SEMENOV, and JEAN FARAGO — Institut Charles Sadron, Université de Strasbourg, CNRS UPR22, France

We have recently discovered that anomalous center-of-mass (CM) diffusion occurring on intermediate time scales in polymer melts can be explained by the interplay of viscoelastic and hydrodynamic interactions (VHI). The theory has been solved for unentangled melts in 3D

[1] and 2D [2] and excellent agreement between theory and simulation is found. The physical mechanism considers that hydrodynamic interactions are time dependent because of increasing viscosity before the terminal relaxation time. We show that this mechanism is generally active and relevant in melts including entangled systems, rings or stars.

[1] PRL 107, 178301 (2011); PRE 85, 051807 (2012). [2] PRL 109, 248304 (2012); *Soft Matter* 9, 4249 (2013).

CPP 49.3 Thu 17:30 ZEU 260

Local Langevin Dynamics in Polymeric Materials — ●DIDDO DIDDENS¹ and ANDREAS HEUER² — ¹Institut Charles Sadron, Université de Strasbourg, 23 Rue du Loess, 67034 Strasbourg, France — ²Institut für physikalische Chemie, Universität Münster, Corrensstraße 28/30, 48149 Münster, Germany

We present an in-depth analysis of the local segmental dynamics in various polymeric materials on the basis of MD simulation data. To this purpose, we employ a Langevin-like, stroboscopic picture of the local chain motion, comprising a systematic, a random and a frictional compound. This concept allows us to extract information about all these individual contributions, thus providing additional insights as compared to conventional observables such as the mean squared displacement. Moreover, due to the entirely local, mode-free approach, this scheme is especially suitable for non-linear polymer architectures or polymers in heterogeneous environments. As a starting point, we compare model systems with different levels of complexity, and assess the influence of the individual parameters. Based on these insights, we turn to simulation data of realistic polymers, and discuss the benefits of our method for a few selected issues in polymer science.

CPP 49.4 Thu 17:45 ZEU 260

Modeling Twin Polymerization processes by ReaxFF — ●THOMAS SCHÖNFELDER¹, JOACHIM FRIEDRICH², STEFFEN SEGER¹, JANETT PREHL¹, and KARL HEINZ HOFFMANN¹ — ¹Department of Physics, Computational Physics, TU Chemnitz — ²Department of Chemistry, Theoretical Chemistry, TU Chemnitz

Twin polymerization is a new synthesis concept which enables the formation of two different macromolecular structures from organo-inorganic hybrid materials in one single process step [1]. It is charac-

terized by two main process types - electrophilic substitutions contributing to the organic network formation and condensation reactions building the inorganic structure for the reviewed monomer 2,2*-spirobi[4H-1,3,2-benzodioxasilene]. To understand the formation process we develop a first-principles-based ReaxFF reactive force field for C/O/H/Si(S,F,Ti,...).

In this work we focus on the required parameters to model the twin-monomer structure and the electrophilic substitution leading to implications on the force field. After extending the ReaxFF model accordingly we are able to present the first steps of the twin polymerization process by molecular dynamics simulations.

[1]: Nanocomposites Prepared by Twin Polymerization of a Single-Source Monomer. S. Grund, P. Kempe, G. Baumann, A. Seifert, S. Spange, *Angew. Chem. Int. Ed.* 2007, 46, 628-632. DOI: 10.1002/anie.200504327

CPP 49.5 Thu 18:00 ZEU 260

Combined methods in Rheology: Rheo-SAXS, Rheo-NMR and Rheo-Dielectric to bridge length and time scales — THOMAS MEINS¹, KYU HYUN^{1,2}, KARL RATZSCH^{1,3}, CHRISTIAN

FRIEDRICH³, BERND STRUTH⁴, and •MANFRED WILHELM¹ — ¹KIT, Karlsruhe, Germany — ²Pusan University, Korea — ³Universität Freiburg, Germany — ⁴Desy, Hamburg, Germany

Rheology as the science of flow and deformation of matter measures in general forces (torque and normal forces) and displacement of materials. Rheology wants to establish the interplay of molecular structure and mechanical properties. Both quantities often differ in their internal length scale starting from 10⁻⁹ m to 10⁻² m and time scales covering 10⁻⁸ s to 10⁺² s. Furthermore mechanical deformation e.g. shear can lead to oriented structures or crystallization if non-linear shear is applied. Consequently there is a need to conduct in-situ molecular characterization techniques during rheological measurements if non-linear shear, e.g. large amplitude oscillatory shear in combination with FT-Rheology is applied.

Within this presentation we would like to present three recent developments within our group to investigate short length scale dynamic measurements (< 1-2 nm) via Rheo-NMR, molecular size (R_g) measurements (ca. 10 * 50 nm) via Rheo-dielectric and structural correlations via Rheo-SAXS measurements. The experimental realization and first experiments will be presented in detail.

CPP 50: Glasses and Glass Transition (joint session with DY/DF) II

Time: Thursday 15:00–17:30

Location: ZEU 114

Invited Talk CPP 50.1 Thu 15:00 ZEU 114

Microscopic investigation of creep in glasses — TATJANA SENTJABRSKAJA¹, PINAKI CHAUDHURI², WILSON POON³, JÜRGEN HORBACH², STEFAN EGELHAAF¹, and •MARCO LAURATI¹ — ¹Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — ²Theoretische Physik II, Heinrich Heine University, Düsseldorf, Germany — ³SUPA and COSMIC, The University of Edinburgh, United Kingdom

The microscopic origin of the creep rheological response of colloidal glasses is investigated, based on the particle-level dynamics measured by confocal microscopy during application of a step stress. Subdiffusive single-particle dynamics are the microscopic signature of creep. At a more local scale enhanced dynamic activity is observed at random locations, with the number of active regions following the time-dependence of the macroscopic strain. Instead, diffusive dynamics characterize the flowing system, with a transient super-diffusive regime during the onset of flow. Transient super-diffusion coincides with the appearance of enhanced dynamics in a specific region of the system, which subsequently rapidly expands and finally spans the whole system when the steady state of flow is reached.

Invited Talk CPP 50.2 Thu 15:30 ZEU 114

Getting into shape: Jamming of frictional particles. — •MATTHIAS SCHRÖTER, JEAN-FRANÇOIS MÉTAYER, FRANK RIETZ, and MAX NEUDECKER — MPI for Dynamics and Self-Organization

In recent years the Jamming paradigm has been promoted as a grand unifying theory of particulate soft matter systems like foams, colloids, emulsions, and granular media [1,2]. However, this approach has mostly evolved from simulations of soft, perfect spheres. Real world particulate systems are often "rough" on either a microscopic or a particle scale. In the first case we talk about friction, in the second about non-spherical shapes.

This talk will use 3D imaging techniques such as X-ray tomography to provide insight into the mechanical stability of tetrahedra packings [3], the volume response of sheared granular media, and the first order phase transition occurring at Random Close Packing. We will show that in non of these three examples the underlying physics is adequately described by the Jamming paradigm.

[1] A. Liu and S. Nagel, *Ann. Rev. Cond. Mat. Phys.* **1**, 347-369 (2010)

[2] M. van Hecke, *J. Phys.: Condens. Matter* **22**, 033101 (2010)

[3] M. Neudecker, S. Ulrich, S. Herminghaus, and M. Schröter, *Phys. Rev. Lett.* **111**, 028001 (2013)

CPP 50.3 Thu 16:00 ZEU 114

Glassy Dynamics of Collapsed Isolated Polymer Chains — •MARTIN TRESS¹, EMMANUEL URANDU MAPESA¹, MANFRED REICHE², and FRIEDRICH KREMER¹ — ¹Universität Leipzig — ²MPI für Mikrostrukturphysik, Halle

While structure and conformation of condensed, isolated low molecular weight and polymeric molecules are well explored, knowledge concerning their dynamics, as measured in a broad spectral range and at widely varying temperatures is sparse. To overcome this, Broad-band Dielectric Spectroscopy is combined with nano-structured electrodes having 35 nm separation and the dynamics of collapsed isolated poly(2-vinylpyridine) (P2VP) globules is measured. The collapsed globule conformation is revealed by Atomic Force Microscopy scans of the identical samples with an average globule volume corresponding to the estimate for a single chain (using the molecular weight and bulk density). Hence, for the first time the dynamic glass transition of condensed isolated polymer chains is directly measured and found to be bulk-like; only segments close (< 0.5 nm) to the substrate are weakly slowed down. The observation of bulk-like dynamics is in full accord with the length scale on which the dynamic glass transition is to be expected. In contrast, the emergence of new, slower relaxation modes is attributed to attractive interactions of the P2VP segments with the supporting silica surface, a finding which is corroborated by complementary infrared experiments. Our approach paves the way for numerous experiments on the dynamics of isolated molecules.

15 min break

CPP 50.4 Thu 16:30 ZEU 114

A direct quantitative measure of surface mobility in a glassy polymer — YU CHAI¹, •THOMAS SALEZ², JOSHUA D. MCGRAW³, MICHAEL BENZAQUEN², KARI DALNOKI-VERESS⁴, ELIE RAPHAËL², and JAMES A. FORREST¹ — ¹University of Waterloo, Canada — ²ESPCI, Paris, France — ³Saarland University, Saarbrücken, Germany — ⁴McMaster University, Hamilton, Canada

The simple geometry of a polymer film on a substrate with a step at the free surface is unfavourable due to the excess interfacial energy induced by the step, thus allowing for a new nanoprobe of the melt state rheology. After recalling the experimental technique, we demonstrate how the same theoretical tools enable to understand the surface evolution of thin polymer films below the glass transition temperature T_g . While above T_g the entire volume between the substrate and the free surface participates to the flow, below T_g only a near surface region responds to the excess interfacial energy. In the latter case, the developed thin film theory for flow limited to the free surface region is in excellent agreement with experimental data. Strikingly, the system transitions from whole film flow to surface localized flow over a narrow temperature region near the bulk glass transition temperature. The measurements and model presented provide a quantitative measure of the surface mobility in a sample geometry where the confinement of polymer chains and substrate effects are negligible. Therefore, this study may help to solve further the ongoing controversy around glass transition in polymer films.

CPP 50.5 Thu 16:45 ZEU 114

Effects of soft confinement on the glass dynamics of glycerol, studied by deuteron NMR — ●MICHAEL LANNERT¹, MARKUS ROSENSTIHL¹, THOMAS BLOCHOWICZ², BERND STÜHN², and MICHAEL VOGEL¹ — ¹Institut für Festkörperphysik, Hochschulstraße 6, 64289 TU Darmstadt — ²Institut für Festkörperphysik, Hochschulstraße 8, 64289 TU Darmstadt

The dynamics of glycerol in a microemulsion with droplet diameters ranging from 2nm to 9nm were investigated by deuteron NMR in the temperature range 150K - 330K. While previous studies of liquid dynamics in confinement mostly used solid matrices, microemulsion droplets formed by AOT surfactants and toluol/m-xylol provide a soft confinement. Deuteron NMR longitudinal (T_1) and transversal (T_2) spin relaxation times, solid echo spectra, and two time correlation functions were recorded. High temperature dynamics are independent from droplet diameter and a Vogel-Fulcher-Tamann temperature dependence was observed. The line shape transition occurs at 240K for all studied droplet sizes, but is broader in confinement than in bulk, indicating a broadening of the distribution of correlation times. Time constants obtained from the measured correlation functions exhibit a weaker, Arrhenius temperature dependence. Detailed analysis suggests that the reorientation results from the rotational diffusion of whole droplets rather than individual molecules.

CPP 50.6 Thu 17:00 ZEU 114

Single molecule diffusion measurements in highly viscous media — ●DOMINIK WÖLL^{1,2} and MAREN DILL² — ¹Zukunftskolleg, Universität Konstanz, D-78457 Konstanz — ²Fachbereich Chemie, Universität Konstanz, D-78457 Konstanz

Single molecule diffusion measurements in highly viscous media require a method which can readily detect very low diffusion coefficients. Single molecule fluorescence tracking typically becomes rather unreliable for diffusion coefficients below $10^{-18} \text{ m}^2 \text{ s}^{-1}$ due to the limited accuracy in determining single molecule positions of a few nanometres and the need for a very high stability of the optical system, even for long-time measurements of several hours. We developed a photocleavable energy transfer dyad which, so far, has allowed us to extend the

range of single molecule (pair) diffusion measurements by three orders of magnitude and to determine slow single molecule motion in polymer films in close vicinity to their glass transition temperature. As a FRET pair, we used a perylene and a terylene diimide derivative, two very efficient and stable fluorophores ideal for single molecule fluorescence spectroscopy. A phenacyl derivative was chosen as the photolabile moiety which could be cleaved with UV light. Initially, the two fluorophores are covalently bound to each other and move correlated before they are cleaved by a UV light pulse and their diffusive separation gives access to low diffusion coefficients of down to $10^{-21} \text{ m}^2 \text{ s}^{-1}$ and beyond.

CPP 50.7 Thu 17:15 ZEU 114

Intermittent Quakes on Surface of Soft Glassy Suspensions — ●TADASHI KAJIYA¹, TETSUHARU NARITA², VELONIQUE SCHMITT³, FRANCOIS LEQUEUX², and LAURENCE TALINI² — ¹Max Plank Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany — ²PPMD-SIMM, UMR 7615 CNRS, UPMC, ESPCI ParisTech, 10 rue Vauquelin, 75231 Paris Cedex 05, France — ³CRPP, UPR 8641 CNRS, Université Bordeaux 1, 115 Avenue Schweitzer, 33600 Pessac, France

We present measurements of the thermal fluctuations of the free surface of oil-in-water emulsions which exhibit a glassy behavior. The Surface Fluctuation Specular Reflection (SFSR) technique was applied to measure the free surface fluctuation. SFSR technique permits to probe the height of the fluctuations of liquid surface using the reflection of a laser beam projected on the target surface [1].

We found that when the volume fraction of the oil droplets is close to or larger than the disordered packing volume fraction, the free surface exhibits abnormal fluctuations, consisting of rare but large amplitude quakes. From a statistical analysis of the fluctuation signal, we also found that such large fluctuations become more prominent as the system ages. These quakes correspond to large changes in the local slope of the free surface over a few tenths of a second. We conjecture that such quakes reflect the dynamics peculiar to glassy systems driven by the relaxations of internal stress [2].

[1] A. Tay et al. Rev. Sci. Instrum. 79, 103107 (2008) [2] T. Kajiya et al. Soft Matter. 9, 11129 (2013).

CPP 51: Charged Soft Matter II

Time: Thursday 15:00–17:00

Location: ZEU 118

CPP 51.1 Thu 15:00 ZEU 118

Temperature-driven structural and morphological changes in multicompartment responsive films — ●SAMANTHA MICCIULLA and REGINE VON KLITZING — Tu Berlin

Responsive coatings are promising candidates to create switchable hydrophilic/hydrophobic surfaces, substrates for cell proliferation/detachment or highly selective uptake/release matrices and still preserve macroscopic properties of the substrate. Polymers are very suitable for this purpose, since many systems can be prepared through simple and well established synthetic routes by varying functionalities and constituent materials. In order to design multifunctional systems, more complex coatings are required. Therefore very recently the combination of grafted and physisorbed polymers has been proposed. Despite structure and properties of each single constituent are known, mutual effects could strongly alter them, hence systematic investigations are required. The mentioned aspects were investigated on a multicompartment matrix made of a thermoresponsive P(NIPAM-*b*-DMAEMA) block copolymer grafted from silica substrate. After quaternization to convert the methacrylate from weak to strong polyelectrolyte, the film is capped with PSS/PDADMAC polyelectrolyte multilayers by dipping. Ellipsometry measurements in water were carried out to monitor the temperature-induced phase transition of the matrix, while Atomic Force Microscopy was used to detect the morphological changes. Finally, the coating of such polymer films by aluminium oxide revealed some fundamental rules governing the interaction between organic and inorganic materials.

CPP 51.2 Thu 15:15 ZEU 118

LCST phase behavior in protein solutions — ●MICHAL BRAUN¹, MARCELL WOLF¹, FELIX ROOSEN-RUNGE¹, FAJUN ZHANG¹, ROLAND ROTH², and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik - Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen —

²Institute for Theoretical Physics - Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen

The phase behavior of BSA and HSA (bovine and human serum albumin) solutions containing yttrium (Y^{3+}) is investigated. For both proteins, a phase diagram in dependence of protein and salt concentration (c_p and c_s) at room temperature has been established ([1], [2]). In a certain regime, the solutions are turbid which is either due to aggregation or liquid-liquid phase separation (LLPS). The 3-D shape of the LLPS binodal for BSA depending on c_p , c_s and temperature T has been measured. A lower critical solution temperature (LCST) phase behavior has been observed. Dynamic and static light scattering measurements are currently performed in order to monitor the diffusion coefficient as well as the static correlation length while the system approaches the binodal. The molecular mechanisms behind this behavior will be investigated in the future, considering the competing effects of ion bridging and hydration.

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

[2] F. Zhang et al., Soft Matter 8 (2012) 1313.

CPP 51.3 Thu 15:30 ZEU 118

Influence of Polycation Molecular Weight on Interdiffusion in Polyelectrolyte Multilayers — ●PETER NESTLER¹, MALTE PASSVOGEL¹, OLAF SOLTWEDEL², RALF KÖHLER³, and CHRISTIANE A. HELM¹ — ¹Inst. f. Physik, Uni Greifswald, 17487 Greifswald, Germany — ²MPI für Festkörperforschung, 70569 Stuttgart, Germany — ³Inst. of Soft Matter and Functional Materials, HZB, Berlin, Germany

For the past twenty years, the Layer-by-Layer technique (LbL) has made it possible to modify surfaces by covering them with thin films. A wide variety of potential applications for polyelectrolyte multilayers (PEM) are demonstrated, for example chemical reactors, antireflective coatings or microcontainers. For all these applications, it is important to control thickness, structure and internal diffusion of the film under

different external conditions.

PEMs are made from poly(diallyldimethylammonium) (PDADMA), poly(styrenesulfonate) (PSS), and deuterated PSS-d. Each film consists of a protonated and a deuterated compartment. The films are annealed in 1 M NaCl and investigated with neutron reflectivity. During annealing the internal interface between both departments broadens due to interdiffusion.

The PSS interdiffusion constant depends non-monotonically on the PDADMA molecular weight, a maximum is observed at 45 kDa, then it decreases by a factor of 3000. The results suggest that PSS and PDADMA move as a complex. Variation of the position of the internal interface as well as the nature of the top layer give insights into the charge distribution within the multilayer films.

CPP 51.4 Thu 15:45 ZEU 118

Rotational Dynamics of Polyelectrolyte Chain Segments Studied by Spin-Label EPR Spectroscopy — ●UWE LAPPAN, BRIGITTE WIESNER, and ULRICH SCHELER — Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Straße 6, 01069 Dresden, Germany

The complex coacervation of oppositely charged polyelectrolytes has been studied by EPR spectroscopy. The spin-label technique employs stable radicals which are covalently attached to diamagnetic macromolecules. Rotational dynamics of such spin labels on time scales between 10 ps and 1 μ s can be characterized by basic and fast CW EPR spectroscopy. The dynamics of the spin labels is influenced by the restricted motion of the side group bearing the label and local polymer backbone motions at the point of the covalent attachment of the label. A spin-labeled poly(ethylene-alt-maleic acid) with less than 5 mol-% of spin-labeled repeat units has been prepared. The segmental rotational mobility of the spin-labeled polyanion and the internal rotation of the spin label have been determined simulating the line shapes of the experimental EPR spectra. The complex formation of this weak polyanion with the strong polycation poly(diallyldimethylammonium chloride) has been studied as a function of mixing ratio and pH of the solution. If the spin-labeled polyanion is the excess component, the spectrum of a slow-motion component is superimposed by the spectrum of a fast-motion component. In the opposite case, the spectra are dominated by a slow-motion component.

CPP 51.5 Thu 16:00 ZEU 118

Ion friction causes current blockades in DNA translocation experiments — ●STEFAN KESSELHEIM and CHRISTIAN HOLM — Institute for Computational Physics, University of Stuttgart, Germany

We investigate the motion of potassium ions and water molecules parallel to the surface of a double stranded DNA molecule under an applied electric field by means of all-atom simulations. Overall we find, that it is described surprisingly well by a simple charged-cylinder model and the electrokinetic equations. The atomistic model, however, exhibits a significant reduction of the ion mobility close to the surface of the DNA, which we interpret as a microscopic friction effect, that is also mediated by the water.

In nanopore experiments the ion current is the main observable. Its modulation by the presence of macromolecules, such as DNA, can be used to infer information about the molecule. Our simulations indicate that the current reduction observed in most experiments is caused by the ion surface friction effect. Our model predicts the crossover electrolyte concentration between current reduction and current enhancement in agreement with experiments.

CPP 51.6 Thu 16:15 ZEU 118

The Hubbard-Onsager dielectric decrement — ●MARCELLO SEGA¹, SOFIA KANTOROVICH¹, CHRISTIAN HOLM², and AXEL ARNOLD²

— ¹University of Vienna, Austria — ²Institute for Computational Physics, Universität Stuttgart, Allmandring 3 70569 Stuttgart Germany

In 1977, Hubbard and Onsager predicted that upon addition of salt to water, the latter should be partly depolarized by an external electric field, resulting in a decrement of the static dielectric permittivity, even though the effect is purely kinetic. This kinetic decrement has never been observed directly, because of the presence of dielectric saturation. Here, we use out-of-equilibrium molecular dynamics simulations to show directly the existence of the kinetic decrement. We show that the kinetic decrement can account to about 10% of the static dielectric permittivity in a NaCl aqueous solution. We compare the simulation results with available theoretical approaches.

CPP 51.7 Thu 16:30 ZEU 118

The Effects of Reactive Oxygen Species on Single Polycation Layers — ●FLORIAN BERG¹, STEFFEN DRACHE¹, STEPHAN BLOCK², REINER HIPPLER¹, and CHRISTIANE A. HELM¹ — ¹Inst. f. Physik, Uni Greifswald, 17487 Greifswald, Germany — ²Chalmers University of Technology, Gothenburg, Sweden

During times of environmental stress (e.g., UV or heat exposure), levels of reactive oxygen species (ROS) can increase dramatically, causing cell damage. Here, the effects of the molecular changes of a polyelectrolyte functionalized surface are investigated.

Positively charged, branched polyethylenimine (PEI) adsorbed onto silicon wafers is 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 μ m 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 radical attacks induce inhomogeneities on the nm-scale.

CPP 51.8 Thu 16:45 ZEU 118

Solvation and ion condensation properties for sulfonated polyelectrolytes in different solvents — ●JENS SMIATEK¹, ANDREAS WOHLFARTH², and CHRISTIAN HOLM¹ — ¹Institut für Computerephysik, Universität Stuttgart, Deutschland — ²Max Planck-Institut für Festkörperforschung, Stuttgart, Deutschland

In contrast to the broad knowledge about aqueous polyelectrolyte solutions, less is known about the properties in aprotic and apolar solvents. We therefore investigate the behavior of sulfonated polyelectrolytes in sodium form in presence of different solvents via all-atom Molecular Dynamics simulations. The results clearly reveal strong variations of ion condensation constants and polyelectrolyte conformations for different solvents like water, dimethyl sulfoxide (DMSO) and chloroform. The binding free energies of solvent contacts with the polyelectrolyte groups validate the influence of different solvent qualities. With regard to the ion condensation behavior, the numerical findings show that the explicit values for the condensation constants depend on the preferential binding coefficient as derived by the evaluation of Kirkwood-Buff integrals. Surprisingly, the smallest ion condensation constant is observed for DMSO compared to water, whereas in the presence of chloroform, virtually no free ions are present.

CPP 52: Biomaterials and Biopolymers (joint session with BP) II

Time: Thursday 15:00–18:45

Location: ZEU 222

CPP 52.1 Thu 15:00 ZEU 222

Observing the onset of amyloid fibril formation at interfaces with Reflection Anisotropy Spectroscopy — ●HEIKE ARNOLDS, SERGIO MAURI, CAROLINE SMITH, and PETER WEIGHTMAN — Surface Science Research Centre, University of Liverpool, Oxford Road, Liverpool L69 3BX, UK

The interaction of proteins with surfaces facilitates misfolding and leads to the formation of amyloid fibrils. This has a major impact on human health, because fibril formation during drug storage and injection decreases drug activity, for example in human insulin, and fibril formation at cell membranes is associated with diseases such as Alzheimer's. The key event is the formation of β -sheet structures which further self-assemble into amyloid fibrils, but there is little mechanistic understanding to date due to a dearth of experimental techniques which are sensitive and informative enough. Reflection anisotropy spectroscopy (RAS) provides structural information of adsorbates from the azimuthal angular variation of the optical spectrum about the direction of the incident light. It has been used for example to monitor the conformational change in cytochrome P450 in real time [1]. Here we apply the technique to the adsorption of human insulin on model methyl and amine terminated stepped Si(111) surfaces. By comparison to attenuated total reflection infrared spectra of the amide I band, we show that RAS can detect a helical β -sheet structure, which likely represents the onset of fibril formation.

[1]P. Weightman et al, Phys Rev E 88, 032715 (2013)

CPP 52.2 Thu 15:15 ZEU 222

UV treatment of stretchable polymer foils for bio-applications — ●RUXANDRA-A. BARB¹, BIRTE MAGNUS², THERESIA GREUNZ⁴, DAVID STIFTER⁴, RAINER MARKSTEINER², SIEGFRIED INNERBICHLER³, and JOHANNES HEITZ¹ — ¹Institute of Applied Physics, Johannes Kepler University Linz, Austria — ²Innovacell Biotechnologie AG, Innsbruck, Austria — ³Innerbichler GmbH, Breitenbach am Inn, Austria — ⁴CDL-MS-MACH, Johannes Kepler University Linz, Austria

Polymers are often used as substrates for cell cultivation. Stretchable polymer foils are required in a cell stretcher, which allows to investigate the behavior of cells during uni-axial mechanical strain or compression [1]. However, many stretchable polymers have weak cyto-compatibility. We demonstrate here that the cyto-compatibility of fluorinated ethylene propylene (FEP) or polyurethane (PU) can be significantly enhanced by UV photo-modification in a reactive atmosphere by means of a Xe2* excimer lamp emitting at 172 nm. Cells seeded on the treated polymer foils show enhanced cell adhesion and proliferation. Water contact angle and XPS measurements indicate that this is a result of improved wettability and a significant change in surface chemistry. However, tensile tests show that UV induced chain scissions can also lead to a degradation of the mechanical stability. But with suitable irradiation dose and foil thickness, repeatedly stretchable polymer foils with sufficient cell adhesion can be prepared.

[1] A. Gerstmair, G. Fois, S. Innerbichler, P. Dietl, E. Felder, J. Appl. Physiol. 107, 613-620 (2009).

CPP 52.3 Thu 15:30 ZEU 222

Mechanics of engineered spider silk microparticles — ●MARTIN PETER NEUBAUER¹, CLAUDIA BLUEM², THOMAS SCHEIBEL², and ANDREAS FERY¹ — ¹Department of Physical Chemistry II, University of Bayreuth, Germany — ²Department of Biomaterials, University of Bayreuth, Germany

Spider silk fibers are well known for their high tensile strength and elasticity. Further, spider silk is biocompatible and -degradable. Thus, application perspectives can be envisaged for pharmaceuticals or cosmetics. Employing recombinant synthesis spider silk proteins are readily available and can be processed into different morphologies such as particles, capsules or films.[1]

We focus on mechanical properties of spider silk microparticles.[2] These could serve as fillers in composite materials or for drug delivery [3]. In this context, the understanding and controlling of mechanics is essential. From AFM force spectroscopy experiments we could show the drastic influence of hydration on the particles' elastic modulus which drops by orders of magnitude. Other investigated parameters include crosslinking and molecular weight. These mechanical studies

are accompanied by the examination of structure, swelling and thermal behavior.

[1] Humenik, M., Smith, A. M., Scheibel, S., Polymers 2011, 3: 640-661

[2] Neubauer, M. P., Bluem, C., Agostini, E., Engert, J., Scheibel, S., Fery, A., Biomater. Sci. 2013, 1: 1160-1165

[3] Bluem, C., Scheibel, T., BioNanoSci. 2012, 2: 67-74

CPP 52.4 Thu 15:45 ZEU 222

Multivalent Ligand Design — ●SUSANNE LIESE — FU Berlin, Berlin

The binding strength of multivalent ligands of different geometry and rigidity is studied, using an analytic statistical mechanics model. By varying the spacer length between the ligand units, the binding strength is optimized. It is found that for low association constants of the monovalent ligand, even an optimized multivalent structure, does not bind better than the monovalent correspondent. The critical association constant above which a multivalent ligand enhances binding, depends cubically on the distance between the receptor binding sites. In all systems we find that a multivalent ligand binds best, if the average spacer length is in the range of the receptor binding site distance and if the spacer is as stiff as possible.

CPP 52.5 Thu 16:00 ZEU 222

Structure/Property-Correlation of Alinate-Surfactant Mixtures at the Water Surface — ●PATRICK DEGEN¹, VICTORIA JAKOBI², MICHAEL PAULUS¹, and METIN TOLAN¹ — ¹Fakultät Physik/DELTA, TU Dortmund, Germany — ²Analytical Chemistry - Biointerfaces, Ruhr-Universität Bochum, Germany

Usually soft colloids, such as emulsion droplets or foam bubbles are stabilized by adsorbed layers of surfactants, polymers and mixtures of both. In recent years industrial researchers focus on polymers that are biocompatible such as gum acacia, chitosan or alginate. Such mixtures are found in pharmaceutical and food applications, in cosmetic products, detergents, and so forth. Nevertheless, the knowledge of basic properties of oil-water interfaces stabilized by surfactant-polymer mixtures is challenged by the complexities of the interactions involved. We present complementary investigations of surface tension and surface rheology properties on the alginate/surfactant system. In combination with dynamic light scattering and fluorescence spectroscopy this work provides new insights into the interactions between alginate and different surfactants in bulk and at the interface. Additionally, X-ray reflectivity measurements give information about the microscopic structure of such interfacial films. We demonstrate that some of the characteristic rheological features related to polymer - surfactant associations correlate with the X-ray reflectivity results, where the formation of large-scale complexes, depending on the surfactant concentration was observed.

CPP 52.6 Thu 16:15 ZEU 222

Determining the Specificity of Monoclonal Antibody HPT-101 to Tau-Peptides with Optical Tweezers — ●TIM STANGNER¹, CAROLIN WAGNER¹, DAVID SINGER², STEFANO ANGIOLETTI-UBERTI³, CHRISTOF GUTSCHE¹, JOACHIM DZUBIELLA³, RALF HOFFMANN², and FRIEDRICH KREMER¹ — ¹University of Leipzig, Department of Experimental Physics I, D-04103 Leipzig, Germany — ²University of Leipzig, BBZ, D-04103 Leipzig, Germany — ³Humboldt University Berlin, Department of Physics, Berlin 12489, Germany

Optical tweezers-assisted dynamic force spectroscopy (DFS) is employed to investigate specific receptor/ligand bindings on the level of single binding events. Here, the binding of the phosphorylation-specific antibody HPT-101 to tau-peptides (pThr231/pSer235) with two potential phosphorylation sites is analyzed. According to ELISA-measurements, the antibody binds only specificity to the double-phosphorylated tau-peptide. It is shown by DFS that HPT-101 binds also to each sort of the mono-phosphorylated peptides. By analyzing the measured rupture-force distributions characteristic parameters are determined for all interactions. Using the extracted bond parameters, we build a simple theoretical model to predict features of the unbinding process for the double-phosphorylated peptide purely based on data on the monophosphorylated ones. Furthermore we introduce a method to estimate the relative affinity of the bonds. The values

obtained for this quantity are in accordance with ELISA, showing how DFS can offer important insights about the dynamic binding process that are not accessible with this common and widespread assay.

15 min. break

Invited Talk CPP 52.7 Thu 16:45 ZEU 222
Threading DNA through nanopores for biosensing applications — ●MARIA FYTA — Institute for Computational Physics, University of Stuttgart

The use of nanopores to read-out in an ultra-fast and cheap way the information inherent in DNA is being intensively investigated the last two decades. A biomolecule, like DNA, in a salt solution is electrophoretically threaded through a nanometer sized pore altering the ionic current that flows through the pore. Simultaneously, measuring the transverse tunneling currents across the nanopore can possibly lead to distinguishable electronic signatures for each DNA unit. Here, we will review some of our work related with the statistical and dynamical characteristics of the translocation process and the ionic current through the pore as obtained through multiscale simulations. Using more accurate simulations we will then report on our attempts to optimize the nanopore. Our efforts are focused on proper functionalization of the nanopore in order to enhance the transverse ionic current for reading-out the genetic information in DNA.

CPP 52.8 Thu 17:15 ZEU 222
DNA Interactions in Crowded Nanopores — NADANAI LAOHAKUNAKORN¹, SANDIP GHOSAL², OLIVER OTTO¹, KAROLIS MISUNAS¹, and ●ULRICH F. KEYSER¹ — ¹Cavendish Laboratory, University of Cambridge, JJ Thomson Ave, CB3 0HE Cambridge, UK — ²Northwestern University, Evanston, IL 60208-3109, USA

The motion of DNA in crowded environments is a common theme in physics and biology. Examples include gel electrophoresis and the self-interaction of DNA within cells and viral capsids. Here we study the interaction of multiple DNA molecules within a nanopore by tethering the DNA to a bead held in a laser optical trap to produce a *molecular tug-of-war*. We measure this tether force as a function of the number of DNA molecules in the pore and show that the force per molecule decreases with the number of molecules [1]. A simple scaling argument based on a mean field theory of the hydrodynamic interactions between multiple DNA strands explains our observations. At high salt concentrations, when the Debye length approaches the size of the counterions, the force per molecule becomes essentially independent of the number of molecules. We attribute this to a sharp decrease in electroosmotic flow which makes the hydrodynamic interactions ineffective.

[1] N. Laohakunakorn, S. Ghosal, O. Otto, K. Misiunas, and U. F. Keyser. DNA Interactions in Crowded Nanopores. *Nano Letters*, 13(6):2798-2802, (2013).

CPP 52.9 Thu 17:30 ZEU 222
Diffusion regulation in the basal lamina — ●FABIENNA ARENDS^{1,2} and OLIVER LIELEG^{1,2} — ¹Zentralinstitut für Medizintechnik, Technische Universität München, Boltzmannstr.11, 85748 Garching — ²Fakultät für Maschinenwesen, Technische Universität München, Boltzmannstr.15, 85748 Garching

The permeability of the basal lamina, a biological hydrogel found at the basolateral side of the epithelium, is an important property for the design of both new drug delivery systems and biomimetic hydrogels. Moreover, it is highly desirable to understand the diffusion of colloidal particles and macromolecules such as drug delivery vehicles, nutrients, growth factors, and proteins across the basal lamina. The mobility of those objects in this highly complex gel is regulated by a broad range of factors including geometric constraints and different types of physical interactions between the particles/molecules and the hydrogel constituents.

Here, we quantify the diffusion of colloids and molecules within an extracellular matrix gel (ECM) purified from the Engelbreth-Holm-Swarm sarcoma, which is a model system for the basal lamina. For this quantification we use single particle tracking techniques and measure the formation of a concentration gradient of solutes across the ECM. From our data we aim at deciphering the underlying mechanisms responsible for the permeability properties of the hydrogel.

CPP 52.10 Thu 17:45 ZEU 222
Induction phase of 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 mechanism which consists of two main processes – DNA replication and segregation. In primitive bacteria such as *Escherichia coli*, which has a rod-like shape and a single chromosome, the dsDNA molecule of the mother cell is split into two daughter strands which are complemented again. During the replication these daughter strands segregate, i.e. move towards opposite sides of the cell to create two new cells. It was previously shown that the segregation of confined linear polymers (DNA) is entropically driven and does not need to involve any active mechanisms [A. Arnold and S. Jun, *Phys. Rev. E* 76 (2007)]. However, the initial configuration of fully overlapping polymers is perfectly symmetrical. Initiation of segregation requires to break this symmetry. This period of time is called induction and has a rather broad distribution, which significantly reduces the efficiency of entropic segregation. In the present study we investigate the induction more closely and determine the mechanism that breaks the symmetry of the system. Combination of MD simulations with theory based on free energy calculation shows that the induction is not diffusive as it was predicted, but is a process related to the ordering of the polymer ends during breaking the system symmetry, when the tail of one strand tries to pass the tail of the other strand. Our findings might explain the segregation delay observed in experiments on *E.coli*.

CPP 52.11 Thu 18:00 ZEU 222
The influence of topology and thermal backbone fluctuations on sacrificial bonds — ●SORAN NABAVI¹, MATTHEW J. HARRINGTON², OSKAR PARIS¹, PETER FRATZL², and MARKUS A. HARTMANN¹ — ¹Institute of Physics, Montanuniversität Leoben, Leoben, Austria — ²Max-Planck-Institute of Colloids and Interfaces, Department of Biomaterials, Potsdam, Germany

One strategy to improve the mechanical performance of natural materials is sacrificial bonding that can be found in bone, wood, and in some softer biological materials like silk, mussel byssus threads. Sacrificial bonds (SBs) are reversible bonds which are weaker than the covalent bonds that hold the structure together. Thus, upon loading SBs break before the covalent bonds rupture. The rupture of SBs reveals hidden length providing a very efficient energy dissipation mechanism. Furthermore, SBs can reform after their rupture providing molecular repair and self-healing. We use Monte Carlo simulations to examine the influence of topology and SBs density on mechanical properties of single polymeric chains. The influence of SB density, topology and thermal backbone fluctuations on mechanical behavior are investigated by computationally mimicking tensile and cyclic loading test. Increasing the SBs density increases the work to fracture and also the energy dissipation in cyclic loading whereas the topology (determines the position and spacing of peak force) and thermal fluctuations (determine height of SB force) changes the mechanical properties. The results bear important implications for the understanding of natural systems and for the generation of strong and ductile biomimetic polymers.

CPP 52.12 Thu 18:15 ZEU 222
Dynamic glass transition in room temperature ionic liquids with calorimetric methods. — ●EVGENI SHOIFET^{1,2}, HEIKO HUTH¹, SERGEY VEREVKIN^{2,3}, and CHRISTOPH SCHICK^{1,2} — ¹Institute of Physics, Rostock University, Rostock, 18051, Germany — ²Interdisciplinary Faculty, Rostock University, Rostock, 18051, Germany — ³Institute of Chemistry, Rostock University, Rostock, 18051, Germany

Many 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.

CPP 52.13 Thu 18:30 ZEU 222
Unusual behavior of vapor deposited glasses of 1-pentene and ethylcyclohexane investigated by fast-scanning and AC chip nanocalorimetry — ●YEONG ZEN CHUA¹, MATHIAS AHRENBERG¹, CHRISTOPH SCHICK¹, KATHERINE WHITAKER², MICHAEL TYLINSKI², and MARK EDIGER² — ¹Institute of Physics, University of Rostock,

Rostock 18051, Germany — ²Department of Chemistry, University of Wisconsin, Madison, Wisconsin 53706, United States

Glasses produced by physical vapor deposition exhibit different densities and relaxation behaviors, depending upon the deposition conditions. Glasses deposited at temperatures of about 0.85 of glass transition temperature T_g , called stable glass, have low enthalpy, low heat capacity, high kinetic stability and high density, while glasses deposited

at much lower temperatures than T_g have opposite properties. We have investigated the glasses of 1-pentene and ethylcyclohexane created from PVD in a wide range of deposition temperatures between 10 K and 120 K by fast-scanning and AC chip nanocalorimetry. Fast-scanning calorimetry provides information about the enthalpy of the deposited samples, while AC chip nanocalorimetry allows for a highly sensitive heat capacity measurement on the same samples.

CPP 53: Organic Electronics and Photovoltaics B (original: DS, joined by CPP, HL, O)

Time: Thursday 17:45–19:45

Location: CHE 91

CPP 53.1 Thu 17:45 CHE 91

The role of residual additives on the stability of polymer blend materials for organic photovoltaic applications. —

•AURÉLIEN TOURNEBIZE^{1,2}, AGNÈS RIVATON², HEIKO PEISERT¹, and THOMAS CHASSÉ¹ — ¹Institute of Physical and Theoretical Chemistry, Tübingen, Germany — ²Institut de Chimie de Clermont-Ferrand, France

Processing additives for improved the morphology of the bulk heterojunction (BHJ) materials used in organic solar cells (OSCs) is now very popular. Thus, by optimizing the donor and acceptor nano domains, the efficiency of OSCs devices could be significantly increased. [1] The impact of those additives on the performances has been widely explored recently but nothing in terms of stability. And yet, a part of the additives stays trapped in the thin film [2] and could participate in the complex photodegradation of the polymer blend materials.

In the present work, we have investigated the impact of residual additives on the polymer blend photostability. By using essentially spectroscopic technics, we have observed an acceleration of the polymer blend photodegradation in presence of additives. In this context, the use of new additives providing a better morphology and by the way a better stability was also explored.

[1] J.K. Lee, W.L. Ma, C.J. Brabec, J. Yuen, J.S. Moon, J.Y. Kim, K. Lee, G.C. Bazan, and A.J. Heeger JACS. 2008, 130, 3619-3623 [2] L. Ye, Y. Jing, X. Guo, H. Sun, S. Zhang, M. Zhang, L. Huo, and J. Hou J. Phys. Chem. C 2013, 117, 14920-14928

CPP 53.2 Thu 18:00 CHE 91

Electronic States and Electrochemical Properties of Polymeric Phthalocyanine Sheets — •CLEMENS GEIS and DERCK SCHLETTWEIN — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany

Phthalocyanines are forming organic semiconducting thin films applicable in field-effect transistors, organic solar cells and as heterogeneous chemical catalysts. They consist of a planar organic aromatic ligand around a central metal atom like *Cu*, *Fe* or *Co*. In a chemical vapour deposition reaction (CVD) phthalocyanines with polymerized ligands were synthesized by reactions of bifunctional 1,2,4,5-tetracyanobenzene with thin metal films. By these means a high concentration of the catalytically active metal-sites on the substrate is established, they are electronically coupled and a molecular network is formed by such sheet polymers. Photoelectron spectroscopy was used to characterize the electronic states of the metals and ligands. Metal ions in the complexes as well as neutral metal clusters were detected in the films. Optical transmission spectroscopy was used to discuss the uniformity of the electronic excitation energy and its dependence on preparation conditions. The films were electrochemically reduced and oxidized to further study their accessible electronic states, study consequences for their optical absorbance and to test the polymeric phthalocyanines as electrocatalysts for water oxidation to oxygen and reduction to hydrogen, reactions of highest interest for the chemical storage of electrical energy from fluctuating renewable sources.

CPP 53.3 Thu 18:15 CHE 91

Asymmetry of mixing length scales and kinetics of phase-separation in co-evaporated donor-acceptor organic thin film blends — •RUPAK BANERJEE, CHRISTOPHER LORCH, ALEXANDER GERLACH, JIŘÍ NOVÁK, CHRISTIAN FRANK, JOHANNES DIETERLE, and FRANK SCHREIBER — Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Small molecular organic semiconductors have found widespread usage in organic photovoltaics (OPV) due to their attractive optical, structural and electronic properties [1]. One of the many ways to tune the

efficiency of an OPV is by mixing donor (D) and acceptor (A) materials [1] since the efficiency depends on the interplay of the diffusion lengths of the excitons generated by the absorption of light and the structural length scales of the D:A mixture. Controlling the structural length scales in D:A mixtures is thus of paramount importance [2]. We discuss *in situ* and real-time x-ray scattering studies on the structure of mixed D:A films as a function of mixing ratio which reveal the kinetics and thickness dependence of phase separation and in particular the asymmetry between top and bottom interfaces [3]. We further discuss the influence of interrupted growth on the phase-separation kinetics of such systems.

[1] W. Brütting and C. Adachi, Physics of Organic Semiconductors, Wiley-VCH, Weinheim (2012).

[2] A. Opitz *et al.*, IEEE J. Sel. Top. Quant. **16**, 1707 (2010).

[3] R. Banerjee, J. Novák, C. Frank, C. Lorch, A. Hinderhofer, A. Gerlach, and F. Schreiber, Phys. Rev. Lett. **110**, 185506 (2013).

CPP 53.4 Thu 18:30 CHE 91

UPS studies on different air-stable molecular n-dopants —

•MARTIN SCHWARZE¹, MAX L. TIETZE¹, PAUL PAHNER¹, BEN NAAB², ZHENAN BAO², BJÖRN LÜSSEN¹, DANIEL KASEMANN¹, and KARL LEO¹ — ¹Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — ²Department of Chemical Engineering, Stanford University, Stanford, California 94305, United States

Understanding the working mechanism of electrical doping in organic semiconductors is essential for the optimization of organic semiconductor devices. A defined doping level allows for the control of the Fermi level position and the conductivity of transport layers. In comparison to molecular p-doping of organic semiconductors, n-doping has the additional problem of air instability. To successfully transfer an electron to the lowest unoccupied molecular orbital (LUMO) of the matrix material, dopants exhibiting shallow highest molecular orbitals (HOMO) are necessary, rendering them prone to reactions with e.g. oxygen. In this study, three different types of n-dopants are compared, an air stable cationic DMBI and DMBI dimer with the air sensitive W2(hpp)4. Doping efficiency, Fermi-level shift, air stability, and conductivity at different doping concentrations are investigated by ultraviolet photoelectron spectroscopy (UPS) and electrical measurements.

CPP 53.5 Thu 18:45 CHE 91

Fracture and corrosion protection for thin-film encapsulation - Fine-tuning the electrical calcium corrosion test for water vapor permeation measurements — •FREDERIK NEHM, HANNES KLUMBIES, LARS MÜLLER-MESKAMP, and KARL LEO — Institut für Angewandte Photophysik, TU Dresden, Dresden, Deutschland

In recent years, the demand for ultra-high moisture barriers has strongly increased due to the ongoing development of organic electronics. Thus, the ability to measure water vapor transmission rates (WVTRs) below $10^{-5} \frac{g(H_2O)}{m^2d}$ - less than a monolayer in 10 days - is crucial for barrier development. The electrical calcium corrosion test - monitoring the decreasing conductivity of a thin calcium film turning into calcium hydroxide - is a sensitive, cost-efficient method to measure such low WVTRs. However, poor design can cause a high background rate or test breakdown. We show that calcium corrosion causes barrier breaking by both expansion and hydrogen emission. As a countermeasure, we introduce organic (C₆₀) buffer layers for decoupling on both sides of the calcium film. Further investigations show elevated calcium corrosion at the calcium-electrode-interface which can be prevented by a proper choice of the electrode material. Finally, the massive corrosion of barrier thin films is shown to be prevented by glueing a polymer foil onto the barrier under testing. With these precautions, we show atomic layer deposited alumina barriers measured in thin film encapsulation.

sulation structure close to an actual device architecture. At 30°C, 90% rh, WVTRs of below $5 \cdot 10^{-5} \frac{g(H_2O)}{m^2 \cdot d}$ were obtained.

CPP 53.6 Thu 19:00 CHE 91

Commensurability as the determining factor for molecular tilt and multilayer growth: In-situ and real-time growth study of the nanographene HBC on SiO₂ and HOPG — ●PAUL BEYER¹, TOBIAS BREUER², SALIOU NDIAYE², ANTON ZYKOV¹, ANDREAS VIERTEL¹, MANUEL GENSLER¹, JÜRGEN P. RABE¹, STEFAN HECHT¹, GREGOR WITTE², and STEFAN KOWARIK¹ — ¹HU Berlin, 12489 Berlin — ²Philipps-Universität Marburg, 35032 Marburg

We investigate the influence of symmetries and the substrate-molecule commensurability on the structure and growth kinetics of the nanographene hexa-*peri*-hexabenzocoronene (HBC). We study organic molecular beam deposited ultrathin HBC films on SiO₂, pristine and sputtered HOPG because of the similar surface energies, singling out the influence of the lattice-matching between HBC and graphite. Using real-time and *in situ* x-ray growth oscillations we find the first ad-layer to grow lying down on both substrates. On pristine HOPG we find a superstructure of hexagonally arranged, recumbent molecules in a new polymorph using GIXD, XRR and NEXAFS. The loss of commensurability in the sputtered HOPG leads to mainly upright molecules. Equally, we find a transition to upright molecules on amorphous SiO₂ surfaces. On SiO₂ micro-crystallites in the bulk structure that completely cover the substrate are found, while the strong ordering on HOPG leads to island growth of the new polymorph as observed by AFM. Our results demonstrate that the (lack of) symmetry- and lattice-matching critically determines the molecular orientation and occurrence of surface induced polymorphs.

CPP 53.7 Thu 19:15 CHE 91

Spray coating process for highly conductive silver nanowire networks as transparent top electrode for small molecule organic photovoltaics — ●FRANZ SELZER¹, NELLI WEISS², DAVID KNEPPE¹, LUDWIG BORMANN¹, CHRISTOPH SACHSE¹, NIKOLAI GAPONIK², LARS MÜLLER-MESKAMP¹, ALEXANDER EYCHMÜLLER²,

and KARL LEO¹ — ¹IAPP, TU Dresden — ²Phy. Chem., TU Dresden
Organic photovoltaics are a promising technology for fabrication in high throughput R2R-coating machines. Therefore, flexible and highly conducting transparent electrodes on temperature sensible polymer films are required. Percolative networks made of silver nanowires (Ag-NWs) are a flexible alternative, showing an opto-electrical performance comparable to ITO. Usually, they are deposited from solution, followed by post-annealing (200°C). The solvents involved in the deposition limit the versatility of this type of electrode and do not allow the direct deposition as top contact onto evaporated small molecule devices. Here, we present a novel spray-coated AgNW mesh, showing excellent opto-electrical performance although processed below 80°C. We investigate different types of wire functionalization and the consequences on typical network parameters of AgNWs. By comparing all investigated materials for different parameters like varying concentration and by scanning electron microscopy, the basics of the sheet resistance reduction mechanism are extracted and AgNW electrodes (<50Ω/sq@>80%) are processed at 30°C. Finally, the successful implementation as transparent top electrode for high-performance organic p-i-n type solar cells is demonstrated.

CPP 53.8 Thu 19:30 CHE 91

Tuning the energy levels of carbon nanotubes by functionalization — ●GERHARD LACKNER¹, WEI XIA², VLADIMIR SHVARTSMAN¹, MARTIN MUHLER², and DORU C. LUPASCU¹ — ¹Institute for Materials Science, University of Duisburg-Essen, 45141 Essen, Germany — ²Laboratory of Industrial Chemistry, Ruhr-University Bochum, 44801 Bochum, Germany

Carbon nanotubes (CNT) are a promising material for electrical applications due to their extraordinary properties. Nevertheless, a defined tuning of the energy levels of this material has not been reported so far. We show a possible route to set the energy levels of CNT by functionalization. The energy levels before and after the functionalization are analysed by Kelvin Probe measurements. Additionally, the functionalized and non-functionalized CNT are applied in organic solar cells and a comparative study about the solar cell performances is given.

CPP 54: Poster Session 3

Transport and Confinement, New Instruments and Methods, Charged Soft Matter, Physics of Food, (Active) Colloids and Complex Liquids, Gels and Elastomers, Nanoparticles and Composite Materials

Time: Thursday 15:00–19:00

Location: P2

CPP 54.1 Thu 15:00 P2

Properties of solvent mixture confined between silica slabs — ●XIANGYANG GUO, TOBIAS WATERMANN, CHRISTOPH ALLOLIO, and DANIEL SEBASTIANI — Institute of Chemistry, Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 4, 06120 Halle (Saale)

Firstly, we investigate the anomalous structure and hydrogen bond network of pure water confined between 2 silanol slabs through ab initio simulations. We compute the proton NMR chemical shifts of confined water as a measure for the strength of the hydrogen-bonding network based on a first principle approach. Our calculations illustrate both the modifications of the 1H NMR chemical shifts of the water with respect to bulk water and a considerable slowing down of water diffusion. Furthermore, we perform classical MD simulations on ethanol-water mixture under confinement using the same silica surface model. The diffusion coefficients of water and ethanol in the confined mixture are reported. The computed density profile shows that evident molecular segregation appears in the confined mixture. Ethanol molecules are more likely to form hydrogen-bonds with silica surface whereas most water exists as small hydrogen-bonded clusters at the center of the pore. This observation is corroborated by the wall-solvents radial distribution functions.

CPP 54.2 Thu 15:00 P2

Simulation of polymer melts in confined geometries — ●ANDRE GALUSCHKO, MARCO WERNER, MICHAEL LANG, and JENS-UWE SOMMER — Leibniz-Institut für Polymerforschung Dresden, Hohe Strasse 6, 01069 Dresden, Deutschland

Polymers in their disordered liquid state show unique viscoelastic properties when the chains start to entangle. The topological constraints created by interchain excluded volume and uncrossability, lead for a

probing chain to move within a tube. We employ the Bond Fluctuation Model to simulate the diffusion dynamics of long polymer chains at melt conditions. When the melt becomes confinement between two ideal walls, the bulk limit is reobtained, when walls separation becomes large compared the free chain extension. With increasing confinement the diffusion accelerates due to change of entanglement density and chain overlap density.

CPP 54.3 Thu 15:00 P2

Fluorescence correlation spectroscopy at reflecting substrates for investigation of vertical sample modulations — ●DANIELA TÄUBER, KATHRIN RADSCHKEIT, MICHAEL SCHULZ, and CHRISTIAN VON BORCZYKOWSKI — Institut für Physik, TU Chemnitz, Germany

Fluorescence correlation spectroscopy (FCS) is widely used for characterization of dynamic material properties [1]. The usually employed confocal laser profiles render a vertical resolution of 1 micron. Reflecting substrates create interference patterns which allow for a vertical modulation of the fluorescence signal [2] in the range of 100-200 nm. Employment of spacer layers [2] and proper choice of excitation wavelength and fluorescent dyes or material properties, therefore, allows for tailored investigation of the vertical modulation of physical properties accessible by FCS. Here we present a modified correlation function for translational diffusion in thin films on reflecting substrates. Boundary effects and long range interactions affect the dynamics of materials and tracer molecules [3], in particular, within highly structured materials such as liquid crystals films [4] and liquid crystalline biomaterials. We apply the presented correlation function to investigate the dynamics of perylenediimides in thin liquid crystal films on silicon wafers with and without a 100 nm thick silica spacer layer.

[1] E.P. Petrov, P. Schuille, Springer Series on Fluorescence.

Springer, 2008, 145-197. [2] A. Lambacher, P. Fromherz, J. Phys. Chem. B 105 (2001) 343. [3] D. Täuber, I. Trenkmann, and C. von Borczyskowski, Langmuir 29 (2013) 3583. [4] B. Schulz, D. Täuber, C. von Borczyskowski et al., Soft Matter 7 (2011) 7431.

CPP 54.4 Thu 15:00 P2

Diffusive mechanism of linear and branched molecules translocation through the "hairy" microchannels — ●IRINA NERATOVA^{1,2}, 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 or "hairy" channels have attracted a lot of attention in recent years for both engineering and biomedical applications. In recent years interest to polymer brush-covered nanochannels is based mostly on microfluidic processes which are intrinsic to living organisms. Many works have been done to understand the processes of opening and closing of the nanochannels. In our project we raise the question about the transport of the molecules through the "hairy" channels. By means of Molecular Dynamics simulations we study the flow dynamics in a microchannel. In particular we investigated the influence of the architecture of macromolecules with the same molecular weight on their ability to pass through a brush-covered channel driven by Poiseuille flow. The simulations indicate that flow conditions cause the speeding up of the transport of molecules with linear architecture through the nanochannel making their velocity comparable with fast but non-draining 30-arms stars. The simulation results reveal that stretching-collapse mechanism of linear molecules in the flow helps to diffuse freely through the pore while the large molecules like 5-, 10-, 15-arms stars are trapped in the channel.

CPP 54.5 Thu 15:00 P2

Segmental Mobilities in Polymer Films — ●DIDDO DIDDENS¹, ANDREAS HEUER², JÖRG BASCHNAGEL¹, and HENDRIK MEYER¹ — ¹Institut Charles Sadron, Université de Strasbourg, 23 Rue du Loess, 67034 Strasbourg, France — ²Institut für physikalische Chemie, Universität Münster, Corrensstraße 28/30, 48149 Münster, Germany

The dynamical properties of polymer chains in thin films as compared to their counterparts in the bulk are of special interest for both practical applications as well as theoretical considerations. Here, we study the local segmental motion in polymer films on the basis of MD simulation data. In particular, we focus on the mobility of a given segment in dependence of its position within the film (i.e. in the center or close to the interface). This is done by our recently developed method [1], which utilizes the Langevin equation to interpret specific averages of the segmental motion in order to yield an effective mobility. Since this approach is purely local, it also allows the extraction of segmental mobilities for polymer chains in confined geometries, thus contrasting the non-local Rouse mode analysis. Additional emphasis is put on the effect of the interface (either a solid wall or vacuum) on the segmental motion.

[1] D. Diddens, M. Brodeck, A. Heuer, EPL 91 (2010) 66005

CPP 54.6 Thu 15:00 P2

Thermotropic Orientational Order of Discotics in Nanochannels: An Optical Polarimetry Study and Landau-de Gennes Analysis — ●MARK BUSCH¹, SYLWIA CALUS², CAROLE V. CERCLIER³, RONAN LEFORT³, DENIS MORINEAU³, BERNHARD FRICK⁴, KRISTINA KRAUSE⁵, ANDREAS SCHÖNHALS⁵, ERIC GRELET⁶, DANIEL RAU⁷, ANDRIY V. KITYK², and PATRICK HUBER^{1,7} — ¹Materials Physics and Technology, Hamburg University of Technology, D-21073 Hamburg, Germany — ²Faculty of Electrical Engineering, Czestochowa University of Technology, 42-200 Czestochowa, Poland — ³Institut de Physique de Rennes, CNRS UMR 6251, Université de Rennes 1, 35042 Rennes, France — ⁴Institut Laue-Langevin, BP 156, 38042 Grenoble Cedex 9, France — ⁵BAM Bundesanstalt für Materialforschung und -prüfung, 12205 Berlin, Germany — ⁶Centre de Recherche Paul-Pascal, CNRS UPR 8641, Université de Bordeaux 1, 33600 Pessac, France — ⁷Experimental Physics, Saarland University, 66041 Saarbrücken, Germany

Optical polarimetry measurements of the orientational order of a discotic liquid crystal (Py4CEH) confined in parallel-aligned nanochannels of monolithic, mesoporous alumina, silica, and silicon as a function of temperature, channel radius (3 - 22 nm) and surface chemistry reveal a competition of radial and axial columnar order. The evolution of the thermotropic nematic order parameter of the confined systems

is continuous, in contrast to the discontinuous transition in the bulk. This behaviour is analyzed by Landau-De Gennes models for discotic order in nanoconfinement.

CPP 54.7 Thu 15:00 P2

Structure and Dynamics of Water in a Porous Silicate: Confinement from First Principles — ●CHRISTOPH ALLOLIO¹, FELIX KLAMETH², and DANIEL SEBASTIANI¹ — ¹Institute for theoretical chemistry, Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 4, 06120 Halle (Saale) — ²Institute for solid state physics, Technical University Darmstadt, Hochschulstr. 6-8, 64289 Darmstadt

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. In order to realistically describe the confinement effects of an amorphous silica pore, we have constructed a fully atomistic model of a such a system using ab-initio molecular dynamics. Pressure and temperature effects on the water structure and thermodynamics, as well as local effects on water mobility have been investigated using both classical and first principles molecular dynamics. We find a considerable slowing down of water diffusion at a water silica interface, accompanied by a change in tetrahedral ordering and weakening of the H-Bond network. Results are in good agreement with predictions from a model interface.[2]

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 54.8 Thu 15:00 P2

Mechanical Characterization of single sub-micron Diameter Fibers via AFM — ●BENEDIKT NEUGIRG¹, DANIEL KLUGE¹, JULIA SINGER², HANS-WERNER SCHMIDT², and ANDREAS FERY¹ — ¹Department of Physical Chemistry II, University of Bayreuth, 95440 Bayreuth, Germany — ²Department of Macromolecular Chemistry I, University of Bayreuth, 95440 Bayreuth, Germany

Many biological and artificial materials are composites with sub-micron diameter fibers as principal building unit. Mechanical characterization on the single fiber level requires advanced probing techniques beyond the standard methods. We utilize the AFM to do nanoscale bending which is applicable to a wide variety of systems. Generally, fibers are deposited on structured glass substrates and investigated in a combined AFM/optical microscope setup. In our contribution we will show results of fiber bending perpendicular and parallel to the substrate plane. We will discuss the advantages of these two bending modes, for example validation of boundary conditions, direct integration of optical methods and the detailed investigation of the mechanical properties beyond linear elastic deformations. Our study focuses on supramolecular fibrillar assemblies of benzenetrisamidines. Although the main intermolecular interaction are hydrogen bonds (in contrast to covalent bonds in classical polymers), these structures show Young's moduli in the GPa range. By varying the molecular structure, stiffness and fiber diameter can be tailored. Besides self-assembly, electrospinning is a complementary preparation route which makes the material accessible via a "Top-down" as well as a "Bottom-up" approach.

CPP 54.9 Thu 15:00 P2

New Developments in Laboratory SAXS Instruments — ●BASTIAN ARLT — Anton Paar Germany GmbH, Ostfildern, Germany
Surfactants, dispersions, polymer or protein solutions and (micro-) emulsions are intensively investigated systems in current science. Consequently, an essential point is the careful characterization of these systems in-situ. The small angle X-ray scattering (SAXS) technique offers precise and fast measurements to investigate parameters such as size, shape, interaction effects of particles in solution. Thus, SAXS is a complementary method to TEM, AFM, or NMR techniques. SAXS measurements are performed at synchrotron facilities or, thanks to recent developments, using laboratory instruments which have become an excellent alternative.

We are going to present the latest developments and trends in the field of laboratory SAXS instruments. Thanks to high-flux X-ray sources, short exposure times are possible. Additionally, Anton Paar has explored novel techniques in sample positioning which are commonly known from synchrotron measuring stations and allow extending the available detection range and to resolving smallest dimensions.

CPP 54.10 Thu 15:00 P2

A high pressure cell for x-ray reflectivity measurements of liquid/solid interfaces and lipid layers — ●PAUL SALMEN, JULIA NASE, BENEDIKT NOWAK, MICHAEL PAULUS, FLORIAN J. WIRKERT, and METIN TOLAN — Fakultät Physik/DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany

We present a high pressure cell for in situ x-ray reflectivity (XRR) measurements[1]. By applying high hydrostatic pressures (HHP) up to 5 kbar, the liquid/solid interface can be studied. The cell consists of two separated parts, an outer cell to withstand the pressure and an inner cell with a separated volume containing the sample. As solid interface, silicon wafers, which can be covered by different coatings, are used.

In the near future, we want to measure adsorption of proteins at lipid layers under HHP. Lipid capsules play a mayor role for example in food processing and drug delivery. To study a simplified system, we spin-coat layers of glycerol tristearate on silicon wafers. Here we present first XRR measurements

[1] F. J. Wirkert et al., *Journal of Synchrotron Radiation* 2014 (21) doi:10.1107/S1600577513021516

CPP 54.11 Thu 15:00 P2

Hybrid GRIN lense microresonator for sensing applications — ●MICHAEL METZGER¹, ANDREAS HORRER², SABRINA RAU¹, GÜNTHER GAUGLITZ¹, DIETER KERN², MONIKA FLEISCHER², DAI ZHANG¹, ALFRED J. MEIXNER¹, and MARC BRECHT³ — ¹IPTC, University of Tübingen, Germany — ²Institute for Applied Physics, University of Tübingen, Germany — ³Zürcher Hochschule für Angewandte Wissenschaften, IAMP, Winterthur, Switzerland

An optical hybrid system consisting of a gradient-index lense (GRIN lense) and a Fabry-Pérot optical microresonator used as a sensitive and compact refractive index sensor is presented. GRIN lenses are miniaturized optical elements, which achieve their focusing effect by a gradient of the refractive index within the lens material. The GRIN lenses enable controlled positioning of the focal plane at one of their flat surfaces. Our microresonator consists of two opposing mirrors - a silver coated GRIN lense and a curved mirror in close proximity ($\lambda/2$ -region). The transmission through the resonator shows a spectrally well-defined Newton ring pattern. The transmission wavelength depends on the mirror spacing and the intra cavity refractive index. The combination of a GRIN lense with a Fabry-Pérot optical microresonator gives us the opportunity to sense smallest changes of the intra cavity refractive index. The reflective layers can be supplemented with an antibody layer to conduct further analytical tests like detection of single macromolecules (e.g. antibody virus bonding) affecting the cavities' dielectric properties. This project was financed by Baden-Württemberg Stiftung.

CPP 54.12 Thu 15:00 P2

Spectroscopy of Dielectric Elastomer Actuators for the Application of Tunable Optical Elements — ●IRMA SLOWIK¹, MARKUS FRANKE², MARKAS SUDZIUS¹, RENE KÖRBITZ², HARTMUT FRÖB¹, ANDREAS RICHTER², and KARL LEO¹ — ¹Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr Str. 1, 01069 Dresden — ²Institut für Halbleiter- und Mikrosystemtechnik, Technische Universität Dresden, Nöthnitzer Straße 64 01187 Dresden

Dielectric elastomers are promising materials for electromechanical systems because of their high dielectric strength and their ability to deform under applied voltage up to very high strains $> 300\%$. Dielectric elastomer actuators are used for artificial muscles, conformable displays, stretchable integrated circuits and biomedical electrode interfaces. Due to their high transparency and flexibility they show a high potential to build up tunable optical elements like tunable phase plates, cavities, or gratings.

We report on a dielectric elastomer film investigated by Fabry-Perot interferometry. The thin polymer film is sandwiched between two compliant ring electrodes. Under applied voltage, the electrostatic force squeezes the dielectric layer, which causes a deformation of the device. The thickness change in the actuator film can lead to a phase change up to several π . Additionally, dielectric elastomer actuator coated with a partly transparent mirror can act as a part of a tunable cavity. Due to the high resolution of the Fabry-Perot interferometer even small changes in the cavity length can be detected.

CPP 54.13 Thu 15:00 P2

Simultaneous Mapping of Long-range Attractive and Short-range Repulsive Forces with MUSIC Mode Atomic Force

Microscopy — ●DIANA VOIGT, EIKE-CHRISTIAN SPITZNER, FABIAN SAMAD, and ROBERT MAGERLE — Chemische Physik, Fakultät für Naturwissenschaften, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

Intermittent contact (IC) or tapping mode atomic force microscopy (AFM) usually focuses on the imaging of the surface morphology and the nanomechanical properties. Beyond that also long-range interactions, like electrostatic and magnetic forces, can be measured with AFM. Multi set-point intermittent contact (MUSIC) mode AFM is based on the point-wise measurement of amplitude and phase of an oscillating AFM tip as the tip-sample distance is reduced. It allows for the determination of the unperturbed height image as well as phase images for a wide variety of amplitude set-points from a single measurement run. Furthermore, the results are not affected from feedback-loop and tip-indentation artifacts. Here, we demonstrate the single-pass measurement of long-range attractive electrostatic and magnetic interactions in addition to the nanomechanical properties of the specimen. As model systems for mapping local differences in the hydrophilic/hydrophobic electrostatic interactions we use PS-b-PEO block copolymer thin films on a silicon substrate and collagen fibrils immobilized on PDMS. As a third example, the nanomechanical properties of a thin film of PS-b-PB block copolymer as well as the magnetic properties of an underlying CoPt thin film are measured in a single run.

CPP 54.14 Thu 15:00 P2

Modular fluidic System for Agglomeration Experiments — ●DOMINIK GERSTNER and TOBIAS KRAUS — Leibniz-Institut für Neue Materialien (INM), Campus D2 2, D-66123 Saarbrücken

Nanoparticles (NP) are used in research and in an increasing number of applications. Agglomeration of their dispersion can occur in every processing step and is often regarded a nuisance. We exploit agglomeration to tune structure and properties of particle-containing nanocomposites [1]. To understand the structure-directing mechanisms, we systematically study the agglomeration of NP having different cores and surfaces. Here, we present a steady-state approach to NP agglomeration studies that uses fluidics and online analysis to improve precision, comparability and throughput. The setup lets us investigate shear effects in nanoparticle processing, too. We combine UV/Vis Spectroscopy and Small Angle X-ray scattering techniques to characterize agglomerates. We discuss experimental challenges that have to be overcome for such flow-based experiments. Proper reagent mixing is crucial, but limited by the laminar flows, and requires careful tuning of flow rates. Agglomerating particles tend to adsorb on the inner walls of the system. We develop strategies to avoid excessive fouling. This contribution shows first results on the tuning of agglomeration states under steady state conditions.

[1] P. Born and T. Kraus. *Phys. Rev. E* 87 (2013), 062313.

CPP 54.15 Thu 15:00 P2

Implementing a OPV slot dye coating device and determining the ramifications on morphology and device lifetimes — ●SEBASTIAN M. GÜNTHER, CHRISTOPH J. SCHAFER, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany

Organic photovoltaics (OPV) represent a highly investigated technology with great advantages in comparison to current PV technologies. Even though recent organic PV devices are reaching efficiencies beyond 10%, there is still a substantial amount of research needed. That regards especially to analysis of morphology, which is a key parameter to efficient devices and also affects degradation as well as device lifetime. Therefore particularly the processing method is of interest as it is expected to have an extensive influence on the morphology. Currently investigated devices are generally processed via spin coating although this technique is not viable for large scale production. Thus the influence of a printing method on the structural characteristics will be investigated on the basis of samples produced by positive shim mask slot dye coating. This coating method for OPVs is a technique that allows for very thin film application provided that a very low viscosity solution (~ 1 mPas) is used. For further investigation a new printing device will be implemented. Thereby created films will be analyzed using X-ray reflectivity (XRR), optical and atomic force microscopy (OM, AFM) and UV/Visible light spectroscopy (UV/Vis). The morphology on a nanometer scale will be probed with grazing incidence wide and small angle scattering methods using X-rays and/or neutrons.

CPP 54.16 Thu 15:00 P2

High frequency laser modulated AC chip calorimeter —

•YEONG ZEN CHUA, EVGENI SHOIFET, and CHRISTOPH SCHICK — Institute of Physics, University of Rostock, Rostock 18051, Germany

Combination of different techniques for heat capacity spectroscopy and temperature-modulated calorimetry (TMDSC) allows the determination of complex heat capacity in a wide frequency range. TMDSC covers a limited frequency range from about 10^{-5} Hz to 0.1 Hz. An AC chip calorimeter gives the possibility to decrease the size of the measured sample, hence increases the sensitivity and frequency range. However, the investigation of the dynamic glass transition is still limited to the frequencies up to a few kHz. A new AC chip calorimeter with laser heating is capable of measuring the glass transition temperature of thin film samples in the frequency range up to 1 MHz. The dynamic glass transition of polystyrene and poly(methyl methacrylate) was studied in the frequency range of 10^{-5} Hz to 1 MHz with different calorimetric techniques.

CPP 54.17 Thu 15:00 P2

Block copolymer based membrane for lithium ion microbatteries — •MAJID RASOOL¹, EZZELDIN METWALLI¹, HANS BEYER², ANNA EBERLE², HUBERT A. GASTEIGER², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching — ²TU München, Chemistry Department, LS Technische Elektrochemie, Lichtenbergstr. 4, 85748 Garching

In the light of an increasing demand on power sources for nanodevices, the nano-scaled lithium based membranes paves the way for new opportunities regarding design and application. The morphology of lithium ion-polymer hybrid films [1] based on P(S-b-EO) block copolymer (BC) electrolyte is investigated using small angle x-ray scattering (SAXS). Additionally, lithium containing BC films are sandwiched between two metal electrodes and the film conductivity at different temperatures and salt concentrations is measured using impedance spectroscopy. The current block copolymer electrolyte consists of both conductive lithium containing PEO domains as well as mechanically stable glassy polystyrene domains. Lithium ion incorporation is found to inhibit the crystallization of PEO block, enhance microphase separation and induce lamella-cylinder morphological transition at high lithium ion content. The correlation between the morphology and ionic conductivity of the current lithium ion-polymer hybrid BC films is employed to put an insight into the mechanisms responsible for the conduction of lithium ions in these systems. [1] E. Metwalli, et al., *Macromol. Chem. Phys.* 212, 1742 (2011).

CPP 54.18 Thu 15:00 P2

Aqueous suspensions of laponite discs under confinement — •MARTIN UHLIG and REGINE V. KLITZING — TU Berlin, Straße des 17. Juni 124 D-10623 Berlin, Germany

Laponite is a synthetic disc-shaped clay and mainly used as a nontoxic rheology modifier, e.g. in coatings, paints or personal care products [1]. In aqueous solution the diameter and thickness of a single disc is 25 nm and 1 nm, respectively. The disc's surface is negatively charged, while the rim is positively charged. The protonation of OH- groups, resulting in positive rim charges, can be tuned by pH. Laponite shows complex ageing behavior, as with time the disc's surfaces and rims approach each other and aggregate due to their opposite charges [1]. This contribution concentrates on the behaviour of Laponite discs in confinement. Nanometer scaled charged systems can show so called oscillatory forces in confinement. These forces are a result of electrostatic repulsion and were reported for silica particles [2] and polyelectrolytes [3]. Oscillatory forces indicate that one layer after the other of diluted charged particles is pushed out of the confinement. Both Thin Film Pressure Balance (TFPB) and Atomic Force Microscopy (AFM) are used to investigate if Laponite solutions under confinement show such a behavior. First results using the TFBP indicate oscillatory forces. Experiments studying the system with AFM and investigating the effect of pH as well as of ion concentration are in progress.

[1] Ruzicka, B. et al.; *Soft Matter*, 2011, 7, 1268-1286

[2] Klapp S. et al.; *Phys. Rev. Lett.*, 2008, 100, 118303

[3] Üzümlü, C. et al.; *Macromolecules*, 2011, 44, 7782-7791

CPP 54.19 Thu 15:00 P2

Self - Sensing Ionic Polymer Metal Composite — •PARISA BAKHTIARPOUR, MASOUD AMIRKHANI, and OTHMAR MARTI — Institute of experimental physics, Ulm university, Ulm, Germany

Integration of sensor and actuating properties of Ionic Polymer Metal Composite (IPMC) have attracted a lot of interest in recent decades.

The electrical response of IPMC to the bending can be used for self-sensing. However, using the self-sensing mechanism of patterned IPMC results into cross talk between sensing and actuating part, which even with shielding cannot be avoided entirely. Additionally, two sections are correlated in which the maximum efficiency on one part lead to the minimum efficiency on the other part. We solve these problems by using a high-frequency and a low-frequency voltage as sensing and actuating signal respectively, on an unpatterned sample. IPMC in the high-frequency can be considered as a variable resistance and in the low-frequency works like an actuator.

CPP 54.20 Thu 15:00 P2

Characteristics of the Hydrogen Bond Network of Water — •MIRIAM JAHN and STEPHAN GEKLE — Biofluid Simulation and Modeling, Universität Bayreuth

The special properties of liquid water originate from its hydrogen bond network. Using molecular dynamics simulations of bulk water we confirm the significant influence of hydrogen bonding on the orientational correlation of the molecular dipoles. While the dielectric permittivity of water is known to depend on these collective orientations of the molecules, it is still unclear which geometric structures communicate such collective effects.

Possible candidates are the loops of bonded molecules that characterize the long-range structure of bulk water. Loops are closed paths of hydrogen bonds, composed of the shortest connections between all participating molecules. Our simulations reveal that most of the loops in bulk water consist of six or seven molecules. We further investigate the influence of interfaces on the water hydrogen bond network. This might be the key to the effect that interfaces have on the dielectric permittivity.

CPP 54.21 Thu 15:00 P2

Dielectric effects of sodium salts in aqueous solution — •KLAUS FRIEDRICH RINNE¹, STEPHAN GEKLE², and ROLAND NETZ¹ — ¹Fachbereich Physik, Freie Universität Berlin, 14195 Berlin — ²Nachwuchsgruppe Theoretische Physik, Universität Bayreuth, 95440 Bayreuth

We present dielectric spectra obtained from equilibrium molecular dynamics simulations of 1 molar aqueous solutions (SPC/E water) of NaF, NaCl, NaBr and NaI. The ion specific static and dynamic effects match experiments results. Additionally, sodium chloride is studied concentration dependently.

The dielectric contribution of the water-polarisation auto-correlation is decomposed into different groups depending on solvation shells and the pair state of the nearest ion. It is shown that even second and third solvation shell water is affected by dielectric saturation leading to a red shift of the spectra compared to bulk water.

Moreover, the contribution of the water-ion polarisation cross-correlation is included leading to a reduction of total dielectric signal by 5-10%. A continuous trend of the cross-correlation with increasing anion size is observed. For the first time the ion pairs are grouped in different ion pair configurations showing that the static equivalent conductance of a contact ion pair is about 50% lower than for ion pairs with larger separation. Furthermore, we show the dynamic ion current auto-correlation contributes about one percent to the total static dielectric constant of the solution.

CPP 54.22 Thu 15:00 P2

Thermodynamic Description of the LCST of Charged Thermoresponsive Copolymers — •JAN HEYDA¹ and JOACHIM DZUBIELLA^{1,2} — ¹Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, Hahn-Meitner Platz 1, 14109 Berlin, Germany — ²Department of Physics, Humboldt-University Berlin, Newtonstr. 15, 12489 Berlin, Germany

The dependence of the lower critical solution temperature (LCST) of charged, thermosensitive copolymers on their charge fraction and the salt concentration is investigated by employing systematic cloud-point experiments and analytical theory. The latter is based on the concept of the Donnan equilibrium incorporated into a thermodynamic expansion of a two-state free energy around a charge-neutral reference homopolymer and should be applicable for weakly charged (or highly salted) polymer systems. Very good agreement is found between the theoretical description and the experiments for aqueous solutions of the responsive copolymer poly(NIPAM-co-EVImBr) for a wide range of salt concentrations and charge fractions up to 8%, using only two global, physical fitting parameters.

In addition, the prediction of salt-specific contribution to LCST

is presented in the framework of so called partitioning concept. Inserted into thermodynamic expansion, a novel interpretation of LCST, and cloud point measurements is revealed. In particular, salt effects on transition thermodynamics are obtained for established polymers; PNIPAM or elastine-like-polypeptides.

CPP 54.23 Thu 15:00 P2

Stimuli-responsive reversible hydrogels from triblock polyelectrolytes and polyampholytes — ●MARGARITA DYAKONOVA¹, MARIA T. POPESCU², CONSTANTINOS TSITSILIANIS², KONSTANTINOS KYRIAKOS¹, SEBASTIAN JAKSCH³, and CHRISTINE M. PAPADAKIS¹ — ¹TU München, Physik-Department, Garching — ²University of Patras, Greece — ³JCNS at FRM II, Garching

We investigate the conformational properties of stimuli-responsive hydrogels from triblock polyelectrolytes PtBA-P2VP-PtBA (PtBA and P2VP are poly(tert-butylacrylate) and poly(2-vinylpyridine) and polyampholytes PAA-P2VP-PAA (PAA is poly(acrylic acid)) where the transitions are due to the neutralization of charged groups [1]. Hydrogels are formed at polymer concentrations as low as 0.4 wt%. The mechanical properties depend strongly on the pH value and the salt content [1].

We focus on the related structural changes of the hydrogels. SANS revealed a dependence of the hydrogel structure of the polyampholyte on charge asymmetry and revealed several transitions with increasing electrostatic interaction. Low charge asymmetry causes the collapse of the chain into a globule dominated by the fluctuation-induced attractions between oppositely charged moieties while at higher charge asymmetry, a network is formed. The latter has been confirmed for the polyelectrolyte system. These results demonstrate the origin of the strong changes in mechanical properties.

CPP 54.24 Thu 15:00 P2

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 phase behavior. Using a multivalent cation, Y^{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 of the RC behavior shows a strong difference. The condensed regime and the LLPS region is much broader for a HSA system and the LLPS boundaries were also shifted to lower salt and protein concentrations (c_p), observed by optical microscopy. The major contribution of this changes can be explained by existence of dimers in BSA solutions, observed by GPC and DLS experiments. Due to the dimers a higher c_p is necessary to achieve the same monomer concentration than without dimers. In addition these will be also interactions between monomer and dimers which will also influence the phase behavior. Using an ellipsoid sticky hard sphere potential for fitting the data, determined by SAXS, the effective interaction was calculated [3]. [1] F. Zhang et al., PRL 101, 2008, 148101; [2] F. Zhang et al., Soft Matter 8, 2012, 1313; [3] M. Wolf et al. J. Mol. Liq., submitted.

CPP 54.25 Thu 15:00 P2

Influence of Polycation Molecular Weight and Diffusion Barriers on Interdiffusion in Polyelectrolyte Multilayers — ●PETER NESTLER¹, MALTE PASSVOGEL¹, OLAF SOLTWEDEL², HEIKO AHRENS¹, RALF KÖHLER³, and CHRISTIANE A. HELM¹ — ¹Inst. f. Physik, Uni Greifswald, 17487 Greifswald, Germany — ²MPI für Festkörperforschung, 70569 Stuttgart, Germany — ³Inst. of Soft Matter and Functional Materials, HZB, Berlin, Germany

After introduction of the Layer-by-Layer technique (LbL) twenty years ago, surfaces were modified by covering them with thin films of different composition. A wide variety of potential applications for polyelectrolyte multilayers (PEM) is known, for example chemical reactors, or microcontainers. For these films, it is important to know how interdiffusion due to external stimuli changes the internal film structure.

PEMs are made from poly(diallyldimethylammonium) (PDADMA), poly(styrenesulfonate) (PSS), and deuterated PSS-d. Each film consists of a protonated and a deuterated compartment. The films are annealed in 1 M NaCl and investigated with neutron reflectivity. During annealing the internal interface between both departments broadens

due to interdiffusion.

A branched polycation layer (PEI) in the film centre serves as a diffusion barrier, and the diffusion constant through the barrier decreases monotonically with PDADMA molecular weight. Without the PEI diffusion barrier, PSS diffuses one to two orders of magnitude faster.

CPP 54.26 Thu 15:00 P2

Synthesis and characterization of polyelectrolyte complexes — ●CHRISTIAN KESSLER — Physikalische Chemie der Polymere, TU Dresden, Germany

Polyelectrolyte complexes formed by Poly(dimethyldiallylammonium chloride) (PolyDADMAC) and poly(maleic acid) with three different copolymers were studied and characterized via light scattering, AFM and viscosity measurements. By varying the ratio of polyanion and polycation as well as the copolymers it was possible to tune properties like surface charge, hydrophilicity, radius, molar mass and overlap concentration. By using different chain lengths of PolyDADMAC two distinct complex structures could be obtained. Oppositely charged polyelectrolytes of roughly the same size resulted in spherical structures, while a size ratio of 1:10 produced needle-like complexes. Removal of the needles revealed additional compact spheres which could be shown by light scattering and AFM measurements. The addition of NaCl resulted in a reduction of the molar mass, radius and the second virial coefficient. Above a salt concentration of 0.03 mol/L these properties increased rapidly.

CPP 54.27 Thu 15:00 P2

Dynamics of wet colloids under mechanical load studied by 3D confocal microscopy — JENNIFER WENZL¹, LAURENT GILSON², ULRICH BRÖCKEL², and ●GÜNTER K. AUERNHAMMER¹ — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²FH Trier, Umwelt-Campus Birkenfeld, Birkenfeld, Germany

Wet colloids are prevalent in many industrial applications, e.g. food processing, or pharmaceuticals. Detailed information of the microscopic behavior of wet colloids is still an open field. The challenge is the 3D visualization on the micro scale of the particle structure and liquid distribution, especially under mechanical deformation.

We present a study on model wet colloids, which can be observed in 3D with confocal microscopy. For a high spatial resolution, the refractive index of all components has to be matched: Silica particles (diameter $7\mu\text{m}$), dispersed in a mixture of an aqueous salt solution, and an organic solvent. Partial hydrophobization of the colloid surface allows us to change the contact angle of liquid-liquid interface, i.e. the interaction of the colloids with the liquid interface. We follow the reorganization of this model wet colloids under mechanical load on a single colloid level and discuss the effects due to capillary bridging.

CPP 54.28 Thu 15:00 P2

Aggregation behaviour of doubly thermo-responsive poly(sulfobetaine-b-(N-isopropylmethacrylamide) diblock copolymers — ●NATALYA VISHNEVTSKAYA¹, VIET HOANG², ANDRE LASCHEWSKY², and CHRISTINE PAPADAKIS¹ — ¹TU München, Physikdepartment, Physik weicher Materie — ²Institute of Chemistry, University of Potsdam

Diblock copolymers consisting of a thermo-responsive poly(N-isopropylmethacrylamide) (P(NIPMAM) block) and a zwitterionic poly(sulfobetaine) (P(SB) block) feature both a lower and an upper critical solution temperature in aqueous solution. This is expected to result in transitions from micelles to unimers to reverse micelles as temperature is increased. The self-organization of the diblock copolymers (P(SPP-b-NIPMAM)) in water can be varied by the addition of an electrolyte, resulting in combined UCST-LCST transitions.

The dependence of the phase transition temperatures in aqueous solution on the electrolyte concentration is investigated by means of turbidimetry. The aggregation behavior in aqueous solution with dual stimuli (temperature and electrolyte concentration) is studied by temperature-resolved small-angle neutron scattering, dynamic light scattering (DLS) and fluorescence correlation spectroscopy (FCS).

CPP 54.29 Thu 15:00 P2

Liquid-liquid phase separation in protein - PEG mixture — SALIBA BARSAUME¹, ●FAJUN ZHANG¹, MICHAEL SZTUCKI², ROLAND ROTH³, and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik, Universität Tübingen, Germany — ²ESRF, Grenoble, France — ³Institut für Theoretische Physik, Universität Tübingen, Germany

We present a combined experimental and theoretical study of the liquid-liquid phase separation (LLPS) in protein-PEG mixture. Bovine gamma-globulin solutions mixed with PEG above a critical volume fraction undergo a LLPS at constant temperature. The partitioning of both protein and PEG has been determined which gives the binodal of LLPS. The critical point of the system has been extrapolated from the tie lines. The critical volume fraction is about 6% which is significantly lower than the theoretical value (13-23%) for colloidal systems with isotropic interaction. The resulting phase boundary is compared with the free volume theory for arbitrary shape (Y-Shape) of protein with a radius of gyration of 6.3 nm and the size ratio of 0.3-0.8 between PEG and protein. Furthermore, small angle X-ray scattering has been employed to determine the effective protein-protein interactions approaching LLPS. The reduced second virial coefficient has been determined for samples at the binodal and near the critical point of LLPS, which is further compared and discussed with the value predicted from colloidal theory.

CPP 54.30 Thu 15:00 P2

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

Within mean-field theory we calculate the scaling functions associated with critical Casimir forces for a system consisting of three spherical colloids immersed in a binary liquid mixture near its consolute point. For several geometrical arrangements and boundary conditions we analyze the effect on the critical Casimir force between a pair of colloids due to the presence of a third one. 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 separations, as well as for temperatures close to criticality.

CPP 54.31 Thu 15:00 P2

Mesoscopic approach to colloidal suspensions — ●APURVA SARKAR and MARCO G. MAZZA — Max Planck Institute for Dynamics and Self-Organisation, Göttingen, Germany

We study the dynamics of a quasi-2D system of colloids, dispersed in a simple background solvent. The dynamics of the surrounding fluid is simulated through Stochastic Rotation Dynamics, which consists of random rotations of particles in a predetermined cell, such that mass, momentum and energy are conserved. In between these discrete time solvent-solvent collisions, the dynamics of the heavier colloidal particles is solved through a classical MD simulation. The colloid-colloid as well as colloid-solvent interactions are modelled via Lennard-Jones potentials, with different sets of interaction radii.

Different transport properties of the system such as self-diffusion coefficient and intermediate scattering factor are obtained from this hybrid MD-SRD code. We study and characterize the phase transitions observed in the system.

CPP 54.32 Thu 15:00 P2

Self assembly of order micro pore structure prepared by water vapor condensation on evaporative polystyrene solution — ●FARID FARAJOLLAHI, MASOUD AMIRKHANI, and OTHMAR MARTI — Institute of Experimental Physics, Ulm University, Ulm, Germany

The condensation of water vapor on the evaporative polymeric solution does produce micro-droplets of water (MDW), which leave their trace on the surface after evaporation of both solvent and water. In the proper condition, polymer and organic solvents can effectively reduce the coalescence rate of MDW and form a self assemble hexagonal structure. The polymeric solution consisted of polystyrene and chloroform mixed with different short-chain alcohols (methanol, ethanol and n-propanol) was studied. At a fixed polystyrene concentration, the order pattern formation initiates at specific concentration for each alcohol and reduced by increasing the length of hydrophobic chain alcohol. The pattern observed only within a certain range of alcohol concentrations, which is wider for methanol and become narrow for longer chain alcohols. For each alcohol, the required concentration for pattern formation has reverse relation to the polymer concentration of the solution. As the hydrophobic part of the alcohol chain becomes longer, higher polystyrene concentration is needed to achieve the micro pore pattern.

CPP 54.33 Thu 15:00 P2

Depletion induced sphere-cylinder transition in C12E5 microemulsion: A Small-Angle X-ray Scattering study — ●MASOUD AMIRKHANI¹, SOHEIL SHARIFI¹, SERGIO FUNARI², and OTHMAR MARTI¹ — ¹Institut für Experimentelle Physik, Universität Ulm, Albert-Einstein-Allee 11 89081 Ulm — ²HASYLAB, Notkestrasse 85, D-22607 Hamburg, Germany

Small-angle X-ray scattering was used to study the mixture of C12E5 (pentaethylene glycolmonododecyl ether)/H₂O/n-decane microemulsion and polyethylene glycol (PEG). The size, shape and the structure factor of the microemulsion were investigated by adding the polymer (PEG) to the mixture. Attractive depletion potential was induced between the microemulsion droplets by the non-adsorb polymer. The range and strength of the attractive potential were changed by varying the molecular weight and concentration of PEG. The forward scattering, $S(0)$, of the spherical microemulsion, declined gradually as the polymer concentration decreased. For PEG with the molecular weight of $M_n = 285-315$, the microemulsion morphology remained spherical, but the main peak of the structure factor moved towards a bigger q . When PEG with molecular weights of $M_n = 2200$ and $M_n = 6000$ were used, a shape transition from spherical to cylindrical was induced in line with increasing polymer concentration.

CPP 54.34 Thu 15:00 P2

Structure and Conductivity of Liquid Crystals having Carbonate Segments — ●ANDREAS EISELE¹, KONSTANTINOS KYRIAKOS², MARGARITA DYAKONOVA², CHRISTINE M. PAPADAKIS², and BERNHARD RIEGER¹ — ¹TU München, Department Chemie, Garching — ²TU München, Physik-Department, Garching

The development of lithium ion batteries with higher capacity and a sufficient safety performance is essential for electric vehicles. It is essential to develop non-volatile and nonflammable electrolytes with good ion conductivity. A new approach is the use of liquid crystalline compounds. Liquid crystals which have ion conducting segments can transport ions efficiently as segregation leads to the formation of nanoscale ion pathways.

We investigated liquid crystalline molecules with a perfluorinated aromatic ring as mesogenic core and a cyclic carbonate as ion conductive moiety. Small-angle X-ray scattering revealed that they form the smectic phase. Spontaneous macroscopic alignment was observed. The influence of lithium salt on the alignment of the molecules and the layer spacing was investigated. The findings were compared with anisotropic conductivity measurements in the smectic as well in the isotropic phase to get new insights into the conductivity mechanism.

CPP 54.35 Thu 15:00 P2

Soret diffusion in ternary organic liquid mixtures — ●MATTHIAS GEBHARDT and WERNER KÖHLER — Physikalisches Institut, Universität Bayreuth, D-95440 Bayreuth, Germany

Soret diffusion or thermodiffusion describes the coupling of the local composition of a mixture to a prescribed inhomogeneous temperature field. While significant progress has been achieved over the last decades both on the theoretical and the experimental side, truly multicomponent systems have hardly been considered so far. It is only recently that the focus of interest has turned from binaries to ternaries, which show already a strongly increased complexity in their diffusion behaviour. We have investigated the system of dodecane, isobutylbenzene and 1,2,3,4-tetrahydronaphthalene by means of a two color optical beam deflection technique. For this system the binary edges are well known in literature and can be used as limiting reference. We have developed a fitting routine to evaluate our experimental data based on the idea of Haugen [1]. Now, we are presenting the first results of our ternary measurements over the entire concentration range.

[1] K. B. Haugen and A. Firoozabadi, J. Phys. Chem. B, 110, pp. 17678-17682 (2006)

CPP 54.36 Thu 15:00 P2

Dynamical properties of finite colloidal clusters — ●ANDRÉ SCHELLA¹, ANDRÉ MELZER¹, CHRISTOPH JULY², and CLEMENS BECHINGER² — ¹Institut für Physik, EMAU Greifswald, 17489 Greifswald — ²tes Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart

Colloidal systems are often regarded as macroscopic atomic systems since they allow a direct access to study matter on the kinetic level by means of video microscopy. When the particle number is low, less than thousand say, the system is said to be finite. Deriving physical properties of finite systems is always challenging, since usually

thermodynamic quantities fail in the limit of low particle numbers. Moreover, volume effects and surface effects are always competing in small ensembles. In our contribution, we study colloidal clusters interacting via tunable magnetic dipole forces. The mode properties of these finite ensembles are derived using an Instantaneous Normal Mode (INM) technique [1]. So far, the INM technique has been successfully applied to dusty plasma clusters [2]. To calculate modes of the system, only instant cluster configurations are needed, thus allowing to use this approach even in overdamped situations. The effect of differently shaped confinements on the cluster dynamics will be discussed. Funding via SFB TR-24 Project A3 and the International Helmholtz Graduate School for Plasma Physics (HEPP) is gratefully acknowledged.

[1] T. Keyes, *J. Phys. Chem. A* 101, 2921-2930 (1997) [2] A. Melzer et al., *Phys. Rev. Letters* 108, 225001 (2012)

CPP 54.37 Thu 15:00 P2

Diffusion of nanoparticles in red blood cell suspensions — ●VERA FORSTER and STEPHAN GEKLE — Biofluid Simulation and Modeling, University Bayreuth, Germany

We investigate the diffusion of nanoparticles near highly deformable red blood cells in comparison with theoretical predictions for rigid walls. In our simulations we use a hybrid model which consists of three different parts. The fluid is modelled via the Lattice Boltzmann method, while molecular dynamics are used for nanoparticles with viscous coupling for fluid-particle interactions. The third part contains the deformation of cell-membranes, whose elastic forces are determined from continuum elasticity theory. The immersed boundary method couples fluid and membranes. We measure diffusion directly by employing the mean-square displacement and indirectly via the particle mobility determined by pulling the particle through the liquid.

CPP 54.38 Thu 15:00 P2

Structure and Phase Transitions in a Series of Triphenylene-Based Discotic Liquid Crystals in the Nanoconfined State — ●CHRISTINA KRAUSE, FRANZISKA EMMERLING, and ANDREAS SCHÖNHALS — BAM Federal Institute for Materials Research and Testing, Berlin, Germany

The structure and phase behavior of a series of discotic liquid crystal based on the triphenylene core (Hexakis [nalkyloxy] triphenylene, HATn; n=5, 6, 10, 12) is studied by means of X-ray Scattering and Differential Scanning Calorimetry (DSC) in the bulk and when confined to self-ordered alumina oxide membranes with different pore sizes. The influence of chain length and confinement on the phase transition is discussed in more detail: In confinement the two phase transitions between plastic crystalline and hexagonal ordered phase at lower and from the latter to an isotropic state at higher temperatures are also observed, but different phase structures close to the wall and in the pore center are evidenced by additional peaks in the heat flow for smaller pore sizes. While the former peaks are independent of the pore size, the depression of the phase transition temperatures of the latter ones can be described by the Gibbs-Thomson-equation. With decreasing pore size for both phase transitions the transition enthalpies decrease. The critical pore size d_{crit} estimated for phase transformation from the pore size dependence of the transition enthalpies for each material increases with increasing chain length.

CPP 54.39 Thu 15:00 P2

Molecular Dynamics of a Discotic Liquid Crystals studied by Inelastic Neutron Scattering — ●CHRISTINA KRAUSE¹, REINER ZORN², BERNHARD FRICK³, and ANDREAS SCHÖNHALS¹ — ¹BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, D-12205 Berlin — ²Forschungszentrum Jülich, Jülich Centre for Neutron Science (JCNS), D-52425 Jülich — ³Institut Max von Laue-Paul Langevin (ILL), B.P. 156, F-38042 Grenoble Cedex 9

Discotic liquid crystals (DLC) consist of a flat and rigid aromatic core and attached flexible aliphatic chains. 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. Dielectric relaxation spectroscopy, quasielastic and inelastic neutron scattering are employed to investigate the molecular dynamics of a homologous series of discotic liquid crystal based on the triphenylene core (Hexakis [nalkyloxy] triphenylene, HATn; n=5, 6, 10, 12) with varying length of the side chain in the bulk state. All materials under study show a boson peak (BP). Therefore, the influence of the length of the alkyl chains on its position and shape is investigated.

With increasing lengths n of the side chains the BP shifts to lower frequencies and gains in intensity. This can be discussed employing a self-organized confinement model, where the confinement is generated by the highly ordered columns to the intercolumnar space, where with increasing n the confinement is weakened.

CPP 54.40 Thu 15:00 P2

Analysis of Particle-Particle Interaction Potentials of Nanoscaled Systems in Aqueous Solutions — ●JULIAN SCHULZE¹, JOHANNES MÖLLER¹, MICHAEL PAULUS¹, JULIA NASE¹, METIN TOLAN¹, and ROLAND WINTER² — ¹Fakultät Physik / DELTA, Technische Universität Dortmund, 44221Dortmund, Germany — ²Fakultät Chemie und Chemische Biologie, Technische Universität Dortmund, 44221 Dortmund, Germany

In previous studies, small-angle X-ray scattering (SAXS) was used to study the intermolecular interaction potential of proteins in aqueous solution under the influence of varying conditions such as pressure, temperature, ionic strength and cosolvents. A non-linear correlation between the strength $J(p)$ of the attractive part of the protein-protein interaction and hydrostatic pressure was found with a minimum at ~ 2 kbar, which is probably related to changes in the water structure. Adding NaCl led to a linear increase of the attractive part of the interaction potential, while adding the osmolyte trimethylamine-N-oxid (TMAO) causes a shift of the minimum of $J(p)$ to higher pressures. In the presented work, the pressure dependent structure factor of Ludox colloidal silica has been determined by SAXS. Spherical nanoparticles offer the advantages of an easy, pressure-independent inner structure and tunable surface properties. The results are compared to results found for the protein lysozyme, and differences and similarities will be discussed. Furthermore, the pressure dependent structure of the solvent itself has been explored by wide-angle X-ray scattering (WAXS).

CPP 54.41 Thu 15:00 P2

Dynamic density functional theory of hard sphere crystals and interfaces — ●MOHAMMAD HOSSEIN YAMANI and MARTIN OETTEL — Institut für Angewandte Physik, Eberhard Karls-Universität Tübingen, Tübingen, Germany

Colloidal hard spheres are an intensely studied model system for studying bulk crystals and crystal-liquid interfaces. Classical Density Functional Theory (DFT) is one of the core theoretical approaches of statistical physics of fluids and crystals, which is able to treat this important system successfully and accurately. Hard-sphere bulk crystals and crystal-liquid interface have been studied using both Monte Carlo simulation and DFT of fundamental measure type (FMT) [1,2]. Density profiles, free energies and crystal-liquid surface tensions compare well between these two approaches. We use dynamical density functional theory (DDFT) to evaluate bulk crystal density profiles and free energies as well as the dynamical behavior of the crystal-liquid interface and related surface tension and compare to available simulation data. In the DDFT approach, we compare the sophisticated FMT and the Ramakrishnan-Yussouff (RY) functional with regard to their numerical efficiency in future applications in describing nucleation processes.

[1] M. Oettel et al, Free energies, vacancy concentrations and density distribution anisotropies in hard-sphere crystals: A combined density functional and simulation study, *Phys. Rev. E* 82, 051404 (2010).

[2] A. Härtel et al, Tension and Stiffness of the Hard Sphere Crystal-Fluid Interface. *PRL*, 108, 226101 (2012).

CPP 54.42 Thu 15:00 P2

Pressure calculation for bidisperse magnetic fluids — ●EKATERINA NOVAK¹, ELENA PYANZINA¹, ELENA MININA^{1,2}, 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 (current place of work) — ³University of Vienna, Sensengasse 8, 1090, Wien, Austria

Magnetic fluids are the systems of magnetic dipolar particles suspended in nonmagnetic liquids. Being a liquid even under the influence of magnetic field, ferrofluids are attractive for theoretical and experimental investigations. Industrially synthesized ferrofluids usually have high degree of polydispersity, i.e. the particle size distribution is rather broad. In the work [C. Holm et al, *J. Phys.: Cond. Mat.* 18 (2006)] it was shown that polydispersity influences microscopic properties of ferrofluids dramatically. Even for bidisperse systems an extensive cluster formation was inhibited by the poisoning effect. Thus, the polydispersity should lead to a change of the macroscopic properties. The present study is devoted to elucidation of the question how polydispersity in-

fluences one of the experimentally measurable macroscopic properties such as pressure of the system. We consider bidisperse systems of magnetic dipolar soft or hard particles as the simplest models of polydisperse magnetic fluid. We employ MD simulations, using ESPResSo, in combination with theoretical calculations of pressure based on the method of diagram expansion. In this way we investigate the influence of polydispersity and dipolar interactions on the compressibility of the system.

CPP 54.43 Thu 15:00 P2

Interferometric measurements of photothermally induced local temperature changes inside solutions of functional gold nanoparticles — ●ALEXANDER NEDILKO¹, MALTE LINN¹, ANNE BUCHKREMER², MARCO SCHÜRINGS³, ULRICH SIMON², ALEXANDER BÖKER³, and GERO VON PLESSEN¹ — ¹Inst. of Physics (IA), RWTH Aachen — ²Inst. of Inorganic Chemistry, RWTH Aachen — ³Inst. of Physical Chemistry, RWTH Aachen

Metal-nanoparticle hybrid systems, such as DNA-gold nanoparticle (AuNP) networks and microgels with AuNP cores, have attracted great interest because of their unique optical properties and their versatile biomolecular and chemical functionalities. Since DNA dehybridization and microgel deswelling are temperature-sensitive, the AuNP hybrid systems can be switched between different states by photothermal heating via irradiation with cw laser light. In order to tailor these systems for possible future biomedical or nano-mechanical applications, it is crucial to investigate the laser induced thermal dynamics in the systems and in their vicinity. In this work, we measure the temperature increase inside different AuNP suspensions on a sub-millimeter length scale with a contact free, interferometric method, by exploiting the temperature dependent change of the refractive index of the solution. By spectrally separating the heating and the probing lasers, we are able to measure the photothermally induced temperature increase with ca. 30mK resolution, while simultaneously following the laser induced switching of the AuNP systems by monitoring the scattered probe laser light intensity.

CPP 54.44 Thu 15:00 P2

Buckling Instabilities of Liquid Crystal Filaments Under Compression Stress — ●TANYA OSTAPENKO¹, SEYYED MUHAMMAD SALLI², ALEXEY EREMIN¹, ANTAL JÁKLI², and RALF STANNARIUS¹ — ¹Institute of Experimental Physics, Otto-von-Guericke-Universität, 39106 Magdeburg, Germany — ²Chemical Physics Interdisciplinary Program and Liquid Crystal Institute, Kent State University, Kent, OH 44242, USA

Elastic buckling of solid rods is a well-known phenomenon. However, liquid rods composed of viscous isotropic non-Newtonian fluids (e.g. silicone oil) will buckle only when the diameter-to-length ratio is less than 0.2 [1]. There have been no reports on how a quasi-one-dimensional structured fluid may behave under compression stress, and to what extent the liquid crystal ordering is important in the resulting dynamics.

We report on the buckling behavior and relaxation dynamics for a variety of liquid crystal filaments under compression stress. The amount of off-axis deflection, or lack thereof, is dependent on both filament size and compression velocity. In contrast to other non-Newtonian fluids, liquid crystal filaments may buckle in multiple locations. Additionally, we observed a relaxation of the buckled material after compression. This indicates that there is some flow of material from the deflected segment into the menisci. We also discuss potential applications for this work.

[1] M. Le Merrer, D. Quéré, and C. Clanet, *Phys. Rev. Lett.* **109**, 064502 (2012).

CPP 54.45 Thu 15:00 P2

Meanfield approach to describe magnetic properties of anisotropic dipolar particles — ●TAISIA PROKOPYEVA¹ and SOFIA KANTOROVICH^{1,2} — ¹Ural Federal University, Lenin av. 51, Ekaterinburg, 620000, Russia — ²University of Vienna, Sensengasse 8, 1090, Wien, Austria

Various specially designed colloidal particles became accessible in experiment. The synthesis of such systems is still a challenge, and one needs reliable predictions for the relationship between the particle parameters (sizes, magnetic-nonmagnetic ratios, shape anisotropy) and the macro properties of large particle systems. Several types of magnetic colloids were synthesized, whose properties differed significantly from those of magnetic spherical single-domain nanoparticles in magnetic fluids. It is convenient to divide “non-standard” magnetic col-

loids into two groups according to their anisotropy. If the anisotropy is related to the particle shape, then for magnetic particles the dipole-dipole interaction remains the same and the anisotropy only affects the steric interactions. Whereas, if the particles retain a spherical shape, however the dipole moment itself is shifted away from the particle centre of mass (anisotropic particles), the dipolar part of the Hamiltonian will change. Here, we focus our attention on the theoretical investigation of magnetic properties of recently introduced sd-particles [Kantorovich et al., *Soft Mater*, 2011] and magnetic Janus particles [Ruditskiy et al., *Soft Mater*, 2013]. We develop a first-order mean field approach to study the magnetization and susceptibility of these systems and verify our theory by comparing to the computer simulations.

CPP 54.46 Thu 15:00 P2

Non-additive resistance for the flow of colloids over two barriers — ●URS ZIMMERMANN, MARCO HEINEN, and HARTMUT LÖWEN — Institut für Theoretische Physik II, Universität Düsseldorf, Universitätsstr. 1, 40225 Düsseldorf, Germany

Ohm's law is one of the most central transport rules stating that the total resistance of sequential single resistances is additive. Using dynamical density functional theory we test additivity of sequential resistances on the scale of individual flowing particles by studying the transport of strongly interacting colloids over two barriers. If the barrier separation is getting comparable to the particle correlation length, the total resistance can be significantly larger or even smaller than the sum of the two individual resistances, depending on the barrier separation and the interaction strength between the particles. This allows to control and tune the total resistance with important applications in microfluidics.

CPP 54.47 Thu 15:00 P2

Active Brownian Motion in Crowded Environment — ●PARMIDA SHABESTARI¹, FELIX KÜMMEL¹, IVO BUTTINONI², and CLEMENS BECHINGER^{1,3} — ¹2. Physikalisches Institut, Universität Stuttgart, Germany — ²Department of Materials, ISA, ETH Zürich, Switzerland — ³Max Planck Institute for Intelligent Systems, Stuttgart, Germany

Artificial active swimmers, i.e. Janus particles, suspended in a critical binary mixture, are capable of a self-diffusiophoretic motion upon illumination. In previous experiments, the dynamics of such swimmers close to walls and periodic arrays of rigid obstacles has been investigated [1]. Here, we investigate the dynamics of active swimmers in the presence of a bath of Brownian particles. Such crowded conditions closely resemble the situation of e.g. bacteria in their natural habitat and thus allows to understand how the interaction of active and passive particles affects the particle dynamics and their density distribution. Depending on the density of the Brownian background particles we observe the formation of metastable channels, whose shape and lifetime strongly depend on the densities of active and passive particles but also on the strength of the propulsion force.

[1] VOLPE G, BUTTINONI I, VOGT D, KÜMMERER H J AND BECHINGER C 2011 MICROSWMIMERS IN PATTERNED ENVIRONMENTS *SOFT MATTER* **7** 8810-5

CPP 54.48 Thu 15:00 P2

Cargo Transport with Active Brownian Particles — ●JANNICK FISCHER¹, FELIX KÜMMEL¹, and CLEMENS BECHINGER^{1,2} — ¹2. Physikalisches Institut, Universität Stuttgart, Germany — ²Max Planck Institute for Intelligent Systems, Stuttgart, Germany

Active Brownian particles are capable of taking up energy from their environment and converting it into directed motion; examples range from chemotactic cells and bacteria to artificial micro-swimmers [1]. One potential application of active Brownian particles is using them as shuttles to transport loads within liquid environments. The central issue is to accomplish effective loading and unloading schemes which are independent of specific interaction forces. Here we suggest a novel mechanism which only requires steric interactions and is based on a U-shaped swimmer which is fabricated by photolithography. By reversing the direction of motion, we expect that a load can be picked up and released easily. Apart from understanding the pickup and release on a microscopic scale, we also want to investigate how such swimmers can lead to the redistribution of passive particles depending on the choice of the applied swimming protocol.

[1] Buttinoni, Ivo, et al. "Active Brownian Motion tunable by light." 2012 *J. Phys.: Condens. Matter* **24** 284129

CPP 54.49 Thu 15:00 P2

Effective temperature of an active microrheological tracer in colloidal suspensions — ●ROBERT WULFERT¹, BORIS LANDER¹, UDO SEIFERT¹, and THOMAS SPECK² — ¹II. Institut für Theoretische Physik, Universität Stuttgart, Germany — ²Institut für Physik, Johannes-Gutenberg-Universität Mainz, Germany

It remains an open issue which classes of non-equilibrium systems can be characterized by an effective temperature in a well-defined and meaningful way. A promising and rather generic approach is to consider the fluctuation-dissipation relation (FDR) for driven systems in a non-equilibrium steady state (NESS). We present numerical results obtained via simulation of colloidal suspensions, which are probed by pulling a single tracer particle with a constant force. For this active microrheological scenario, we determine conditions under which the velocity-force FDR becomes approximately time-independent. It can then be interpreted as an effective temperature, accounting for the tracer dynamics on all timescales with a unique value that is equal to the kinetic temperature. Furthermore, we discern in how far the effective temperature depends on the choice of observable by analyzing the anisotropic properties of the tensorial velocity-force FDR.

CPP 54.50 Thu 15:00 P2

Thermoresponsive switching behavior in thin films of cyclic and linear PNIPAM — ●DAVID MAGERL¹, XING-PING QIU², FRANÇOISE M. WINNIK², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — ²Université de Montréal, Faculty of Pharmacy and Department of Chemistry, CP 6128 Succursale Centre Ville Montréal QC H3C 3J7, Canada

Stimuli-responsive hydrogels are a widely studied field of polymers with a huge potential of applications such as drug-delivery systems and sensors. Among this type of polymer PNIPAM is a well-known representative as a model system of a thermo-responsive polymer. It has been shown by comparative studies of linear and cyclic PNIPAM that a cyclic topography of the polymer greatly influences the switching behavior [1]. Within the scope of this study the properties of spin-coated thin films of linear and cyclic PNIPAM with well-defined molecular weights and different film thicknesses are investigated. Film swelling, when exposed to water vapor, and the switching behavior under a thermal stimulus is investigated. Due to the confinement by the substrate no uniform (3D) swelling but a 1D swelling that results in a thickness change of the films is observed by white-light interferometry and further analyzed.

[1] X.-P. Qiu, F. Tanaka, and F.M. Winnik, *Macromolecules* 2007, 40, 7069 - 7071

CPP 54.51 Thu 15:00 P2

Networks from amphiphilic star block copolymers — ●XIAOHAN ZHANG¹, KONSTANTINOS KYRIAKOS¹, MARIA RIKKOU-KALOURKOTI², ELENI N. KITIRI², COSTAS PATRICKIOS², and CHRISTINE M. PAPADAKIS¹ — ¹TU München, Physik-Department, Garching — ²University of Cyprus, Nicosia, Cyprus

Amphiphilic conetworks comprise hydrophilic and hydrophobic chains which microphase-separate when swollen with water. This way, a large amount of internal interfaces is created which is of interest for, among others, tissue engineering. Using end-functionalized star block copolymers for their synthesis results in model networks with low defect density.

We investigate amphiphilic conetworks from various acrylic blocks which differ in composition, water solubility and mechanical properties. Their degree of swelling in water depends strongly on these characteristics. We study the structures of these conetworks using small-angle X-ray scattering which reveals information about the microphase-separated morphology.

CPP 54.52 Thu 15:00 P2

Star-PEG-Heparin-Polyelectrolyte-Hydrogels - Rate Theory and Reaction Kinetics — ●RON DOCKHORN^{1,2} and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden e.V., D-01069 Dresden, Germany — ²Technische Universität Dresden, Institut für Theoretische Physik, D-01069 Dresden, Germany

We are studying biohybrid hydrogels made of heparin, a rod-like highly charged glycosaminoglycan as a highly functionalized cross-linker, and non-charged, elastic 4-arm star-shaped-polyethylene glycol by using theory and simulations. We focus on the network structure and reaction kinetics by using the bond-fluctuation simulation method and

determine the higher order defects at different initial conditions comparing to the rate theory. Also, we investigate the influence of the initial molar ratio, the variations of functionalized groups, and the concentration dependence of the reaction mixture on the reaction kinetics of the defects and on the percolation threshold of the gels. These findings are useful to optimize the mechanical properties of this biohybrid hydrogels for cell replacement-based therapies.

CPP 54.53 Thu 15:00 P2

Polyelectrolyte-4-Arm-Star-Shaped Hydrogels - Swelling Behavior in Different Solvent Conditions — ●RON DOCKHORN^{1,2} and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden e.V., D-01069 Dresden, Germany — ²Technische Universität Dresden, Institut für Theoretische Physik, D-01069 Dresden, Germany

We are studying hydrogels made of charged 2/4-functional point-like cross-linker, and non-charged, elastic 4-arm-star-shaped polymer in solutions of various salt concentrations. We focus on the swelling behavior by using the bond-fluctuation simulation method with electrostatic interaction. We apply both the explicit Ewald summation and the Debye-Hückel-approximation. A mean-field type model is used which combines the effects of counterions and excluded volume to understand the swelling properties of the gels and is compared to the simulation data.

CPP 54.54 Thu 15:00 P2

Laser Heated Nanoparticles in a Thermoresponsive PNIPAM Polymer — ●MICHAEL ORLISHAUSEN and WERNER KÖHLER — Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth

Thermoresponsive polymers have gained wide attention in large areas of polymer physics and physical chemistry. We have investigated laser-heated gold nanoparticles (GNPs) in aqueous solutions of Poly-N-Isopropylacrylamide (PNIPAM) by means of optical microscopy. Gold colloids with radii of 125nm show high absorption around 532nm due to their plasmon resonance. Hence they can be used as effectively point-like heat sources, well below the diffraction limit. We have found that for small laser powers a circular two-phase region grows around the GNP, whose radius grows linearly with increasing power. Due to high surface temperatures well above 500K, a solvent-bubble, which is stabilized by Marangoni-convection, forms around the GNP. In our experiments, we have found that the estimated temperature on the surface of that bubble fits the calculated boiling point of water when taking the Laplace-pressure inside the bubble into account. At constant heating power the two-phase-region also shows a time evolution that can potentially be described on the basis of a demixing delay that depends on the local temperature difference to the critical temperature.

CPP 54.55 Thu 15:00 P2

Hybrid particle of gold nanoparticles embedded in thermoresponsive microgels — ●MAREN LEHMANN, SARAH T. TURNER, LUCAS KURTHS, and REGINE VON KLITZING — Stranki-Laboratory, Dept. of Chemistry, TU Berlin, Germany

For applications such as sensory and drug delivery systems, microgels with the ability to reversibly switch between a collapsed and expanded state in response to an external stimulus (pH, temperature), are attractive. Embedding metal nanoparticles into microgels can introduce new functionalities and enlarge the field of application to catalysis, medicine and nanoreactors [1] [2] [3]. There are different approaches to prepare hybrids of gold nanoparticles and microgels. Lu et al. demonstrated an in situ synthesis of Au-Pt nanorods in core-shell microgel particles by growing rods from gold seeds previously immobilized in the microgel network [4]. We embed gold nanospheres into PNIPAM microgel networks via various mixing routes in order to reach evenly loaded microgel particles. The differently prepared hybrid particles were compared regarding their zeta potential and volume phase transition depending on the temperature. Transmission electron microscopy images were used to evaluate the distribution and loading. The microgel particles were synthesized in a semi-batch method and with positively and negatively charged initiator molecules.

[1] K. Gawlitza et al. *Phys.Chem.Chem.Phys.* 15, 37 (2013). [2] M. Karg et al. *Curr. Opin. Colloid Interface Sci* 14, 6 (2009). [3] H. Lange et al. *Langmuir* 28 (2012). [4] Y. Lu et al. *ACS Nano* 4, 12 (2012)

CPP 54.56 Thu 15:00 P2

molecular dynamics simulation of the LCST shifting of modified PNIPAM — ●YONGBIAO YANG¹, GANESH BALASUBRAMANIAN²,

MICHAEL BÖHM¹, and FLORIAN MÜLLER-PLATHE¹ — ¹Alarich-Weiss-Str. 4 64287 Darmstadt — ²Iowa State University Ames, IA 50011, USA

The local conformation of chemical systems containing photo-responsive units such as spiropyran and merocyanine can be changed by light radiation of suitable wave length. Such photo-responsive units can be added to polymer chains which then become photo-responsive, too. As a result, the functionalized polymers can exhibit reversible functionalities. Poly(N-isopropylacrylamide) (PNIPAM) is a intensively used temperature-responsive polymer with the lower critical solution temperature (LCST) of 305 K. By grafting with merocyanine or spiropyran units, LCST of PNIPAM is expected to be changed. In our simulations, the temperature-responsive behaviour of modified PNIPAM is studied by using molecular dynamics simulations. All-atom models of modified PNIPAM in solution are built based on the parameters obtained from density functional calculations, and molecular dynamics simulations are performed for systems including a single polymer chain. The LCST of PNIPAM is found to be shifted after grafting photo-responsive units. But the influence of merocyanine and spiropyran units are very different. This originates from their different local structures according to our density functional calculations.

CPP 54.57 Thu 15:00 P2

Wetting induced structure formation in elastic porous media — ●ZRINKA GATTIN, OHLE CLAUSSEN, STEPHAN HERMINGHAUS, and MARTIN BRINKMANN — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Göttingen, Germany

When a deformable material is brought in contact with more than one fluid phase, the interplay between the elasticity and interfacial stresses can give rise to unexpected phenomena.

Motivated by experiments on the demixing of binary liquids in polymer gels we study the formation and interaction of liquid droplets in a 2D elastic medium. The phase separating liquids are represented with a lattice gas model, where the elastic matrix is introduced through a network of tethered particles having different affinities to the fluid phases. Our simulations show how the growth of the domains can be inhibited by the elastic medium, altering the dynamics and giving rise to characteristic patterns. The results are compared to predictions of a simple continuum model of the elastic matrix.

CPP 54.58 Thu 15:00 P2

Measurement of microviscosity in crosslinked polyacrylamide-ferrohydrogels by Mössbauer spectroscopy — ●JOACHIM LANDERS¹, LISA ROEDER², ANNETTE SCHMIDT², and HEIKO WENDE¹ — ¹Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg -Essen, Germany — ²Department Chemie, Institut für Physikalische Chemie, Universität zu Köln, Germany

Several polyacrylamide (PAAm) hydrogels with different amounts of methylenbisacrylamide (MBA) crosslinker were prepared, containing acicular hematite (α -Fe₂O₃) nanoparticles. These were used as probes allowing us to examine the local dynamic properties by ⁵⁷Fe-Mössbauer spectroscopy in systems with different degrees of cross-linkage. While static sextet spectra can be observed up to 265K, the width of the sextet lines increases dramatically near the water melting point in all samples, verifying movement of the nanoparticles when the hydrogel approaches the liquid state. This reveals that, contrary to expectations, embedded nanoparticles are not completely immobilized even in strong crosslinked hydrogel networks with us being able to quantify the effects of Brownian motion by Mössbauer spectroscopy. Theoretical calculations allow to estimate the temperature dependent microviscosity ν , which exceeds ν_{H_2O} by far and is correlated to the amount of MBA crosslinker. (This work was supported by DFG WE2623/7-1, SPP1681)

CPP 54.59 Thu 15:00 P2

Smart surfaces from stimuli-responsive microgels via spin coating — ●JOHANNES BOOKHOLD, BASTIAN WEDEL, and THOMAS HELLWEG — Universität Bielefeld, Universitätsstraße 25, Bielefeld, Germany

Stimuli-responsive nano- and microgels are in the focus of interest for a number of applications, such as sensors, drug-delivery and surface coatings. Among these colloidal particles temperature responsive microgels based on poly(n-isopropylacrylamide) (pNIPAm) are the most intensive studied systems. These microgels exhibit a reversible volume phase transition (VPT) at a temperature near the lower critical solu-

tion temperature (LCST) at about 305 K. For most applications a huge advantage of pNIPAm based microgels is that their properties and the external stimuli they respond to can be modified via copolymerization. The resulting properties of the particles can be predicted depending on the used comonomer. The production of coatings and thin films with tailor-made properties from microgels is especially interesting for applications in medical and biological research.

A general, reliable, fast and easy production process for thin films and surface coatings consisting of such microgels is a desirable goal. One already well established method in the field of surface coatings that can offer these features is spin coating. Therefore the access to a variety of microgel coatings and films showing different properties via spin coating is within the focus of this work. Manufactured coatings were characterized using ellipsometry, atomic force microscopy (AFM) and scanning electron microscopy (SEM).

CPP 54.60 Thu 15:00 P2

Characterizing the crosslinking process of PDMS with Rheometry — ●RUDOLF HASSLACHER and SABINE HILD — Institute of Polymer Science, Johannes Kepler University of Linz, Altenberger Strasse 69, 4040 Linz, Austria

Depending on the desired features the wide variety of polydimethylsiloxanes (PDMS) types with different properties (viscosity, hardness, elongation modulus) and applications makes it necessary to select the used type properly. Additionally, knowledge about the crosslinking behavior of PDMS is very important for scientists dealing with it or its composites. During this work different types of PDMS were investigated to find a fully crosslinked PDMS with the desired properties. Therefore the crosslinking behavior was examined with Rheometry. The rheological measurements were carried out with an ANTON PAAR UDS 200 Rheometer. There are different ways of following the curing via Rheometry, namely strain-controlled time resolved frequency sweeps (= time-resolved mechanical spectroscopy = TRMS) and stress-controlled time tests. The TRMS measurements were done at a frequency range between 0.1 and 100 rads⁻¹ (both at 25°C), the stress-controlled tests with constant stress = 75 Pa and constant frequency = 1 Hz. We found a reasonable accordance between these two ways. Through the rheological data we gain the parameters after which we can select the appropriate PDMS for our application.

CPP 54.61 Thu 15:00 P2

Vulcanized fiber studied by x-ray diffraction — ●KARIN RÜSTER¹, DOMINIK DUMKE², MICHAEL PAULUS¹, CHRISTIAN STERNEMANN¹, JULIA NASE¹, JOHANNES MÖLLER¹, KOLJA MENDE¹, IRENA KIESEL¹, DOROTHEE WIECZOREK², and METIN TOLAN¹ — ¹Fakultät Physik / DELTA, Technische Universität Dortmund, D-44221 Dortmund, Germany — ²Fakultät Maschinenbau, Technische Universität Dortmund, D-44221 Dortmund, Germany

Vulcanized fiber is a material of various applications, for example it is used as an insulator in the electrical industry or in welding shields. As it is made from renewable resources, it gained increasing interest in recent years. There are two ways to produce vulcanized fiber: mercerisation and parchmentising. The raw paper is soaked with alkaline (mercerisation) or acidic solution (parchmentising) respectively, pressed to interconnect the layers, rested for a certain time, and washed out in steps of descending concentrations. During this process the material's properties change. The material becomes harder, stiffer, and thicker due to multiple layering and structural changes. The corresponding microscopic mechanisms are analysed by x-ray diffraction (XRD). The raw paper consists mostly of cellulose I_α and I_β, which transforms to cellulose II during the process of mercerisation. The structural changes during the process of parchmentising by zinc chloride were examined. The experiment was performed at beamline BL9 of the synchrotron light source Delta, Dortmund.

CPP 54.62 Thu 15:00 P2

Hydration and molecular interactions in PNIPAM films probed with FTIR spectroscopy — ●ALFONS SCHULTE^{1,2}, MARTINE PHILIPP¹, CHRISTOPH SCHAFER¹, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching — ²Physics Department and College of Optics and Photonics, University of Central Florida, Orlando, FL 32816-2385, USA

The properties of bound water are of considerable interest for hydrogels and their LCST-type demixing transition. Poly(N-isopropyl acrylamide) (PNIPAM) is among the thermoresponsive polymers well studied in solution. In the present investigation we study molecular

changes in PNIPAM films as a function of hydration employing FTIR spectroscopy. PNIPAM films with thickness over the range from 50 to 200 nm are prepared by spin coating on silicon substrates. The infrared spectrum in the CH, OH, and amide band regions provides details on the changes in conformation and hydrogen bonding. These are investigated during a heating-cooling cycle and the time evolution of water storage in the hydrogel films.

CPP 54.63 Thu 15:00 P2

In Situ particle degradation of hyperbranched polyglycerol particles via Atomic Force Microscopy — ●MARCEL RICHTER and REGINE VON KLITZING — TU Berlin, Straße des 17. Juni 124, 10623 Berlin

During the last decades hyperbranched polymers made of polyethylene glycerol (PEG) have attracted much interest in applications like drug delivery and sensors [1]. Due to their biocompatibility and multifunctionality these particles afford the formation of efficient drug carriers [2]. The drug loading with these particles can be realised by the encapsulation during the particle synthesis. This guarantees a homogenous drug distribution within the carrier. The drug release can be triggered by the particle degradation in response to biological stimuli such as changes in pH [3]. The particle degradation has been followed by atomic force microscopy (AFM) as a function of time. It has been found that particle erosion occurs with an exponential decay within the first minutes. Further progress in the degradation process leads to a slow down of the particle erosion. On the other hand, the particle degradation in bulk shows linear particle erosion. [1] *R. Haag, F. Kratz, *Angew. Chem. Int. Ed.* (2006), 45, 1198 [2] K. Knop et al., *Chem. Int. Ed.*, (2010), 49, 6288 [3] *E. Fleige et al., *Adv. Drug Deliv. Rev.* (2012), 64, 866

CPP 54.64 Thu 15:00 P2

Using small angle neutron scattering and light scattering to investigate thermoresponsive copolymer microgels — ●BASTIAN WEDEL, JOHANNES BOOKHOLD, and THOMAS HELLWEG — Universität Bielefeld, Universitätsstraße 25, Bielefeld, Germany

Temperature responsive microgels undergo a volume phase transition (VPT) at a certain temperature (VPTT). It is this specific property that makes such kind of structures interesting for various applications, such as sensors, nanoactuators or as drug delivery systems. An optimal performance of microgels requires a method for an adjustment of the application-specific properties. A suitable and easy method is constituted by the copolymerization of different monomers.

We present a study dealing with the investigation of the physical and structural properties of copolymer microgels based on different temperature responsive alkylacrylamide derivatives with consimilar structures. The used monomers are *N*-*n*-propylacrylamide (NNPAM), *N*-isopropylacrylamide (NIPAM) and *N*-isopropylmethacrylamide (NIP-MAM) with VPTTs of the homopolymer microgels of 22 °C, 32 °C and 43 °C respectively.

We analyzed the dependence of the feed composition and the surfactant concentration in the reaction solution at various temperatures to get an insight into the structural changes during the volume phase transition. Photon correlation spectroscopy and static light scattering were used to investigate the swelling behavior and the overall structure. Furthermore, we performed small angle neutron scattering experiments to clarify the structure on the lengthscale of the polymer network.

CPP 54.65 Thu 15:00 P2

Charge Storage in β -FeSi₂ Nanoparticles — ●JENS THEIS¹, SEBASTIAN KÜPPER¹, ROBERT BYWALEZ², HARTMUT WIGGERS², and AXEL LORKE¹ — ¹Fakultät für Physik and CENIDE, Universität Duisburg-Essen — ²Institut für Verbrennung und Gasdynamik and CENIDE, Universität Duisburg-Essen

The increasing use of mobile electronics creates a steady demand for new energy storages with very high capacitance. Here we report on the observation of a surprisingly high specific capacitance of β -FeSi₂ nanoparticle layers.

Lateral, interdigitated capacitor structures were fabricated on thermally grown silicon dioxide and covered by FeSi₂ particles by drop or spin casting. The FeSi₂-nanoparticles, with sizes in the range of 10-30 nm, were fabricated by gas phase synthesis in a hot wall reactor. Compared to the bare electrodes, the nanoparticle-coated samples exhibit a 3-4 orders of magnitude increased capacitance. Time-resolved current voltage measurements show that for short times (seconds to minutes), the material is capable of storing up to 1 As/g at voltages of around 1 V. The devices are robust and exhibit long term stabil-

ity under ambient conditions. The specific capacitance is highest for a relative humidity of 95%, while for a relative humidity below 40% the capacitance is almost indistinguishable from a nanoparticle-free reference sample.

The devices work without the need of a fluid phase, the charge storing material is abundant and cost effective, and the sample design is easy to fabricate.

CPP 54.66 Thu 15:00 P2

In-Situ Observation of Wrinkle-Formation via UV/Ozone Oxidation — ●BERNHARD GLATZ¹, MORITZ TEBBE¹, ANDREAS SCHEDL², and ANDREAS FERY¹ — ¹Department of Physical Chemistry 2, University of Bayreuth, Universitätsstraße 30, 95447 Bayreuth, Germany — ²Department of Macromolecular Chemistry 1, University of Bayreuth, Universitätsstraße 30, 95447 Bayreuth, Germany

Wrinkled surfaces are versatile tools on the micro- and nano-range, e.g. in their use as photonic crystals or for particle alignment. They can be formed by straining soft substrates that are coated with a thin hard film. The wavelength and amplitude of the resulting periodic surface deformations strongly depends on processing conditions, the thickness of the thin film and mechanical properties of film and substrate. Wavelengths between sub-micron and macroscopic range are accessible, however defect structures like cracks and wrinkle branches are inevitable side features in wrinkling processes and furthermore non-predictable yet.

To better understand defect formation, we developed a setup, which allows observation an in-situ view of currently forming waves and their defect structures via Light Microscopy. We applied the system for investigation of defect formation in systems, which possess defined gradients in elastic constants [1]. We find that rather than appearing in a random fashion, branching defects become ordered and we discuss implications of this finding for the formation of hierarchical structures.

[1] K. U. Claussen, M. Tebbe, R. Giesa, A. Schweikart, A. Fery and H.-W. Schmidt, 2012, *RSC Advances*, 2 - 27, 10185 - 10188

CPP 54.67 Thu 15:00 P2

Response of gold nanorods in solution to external electric fields — ●CHRISTINA LEDERLE¹, DANIEL SCHEID², MARKUS GALLET², and BERND STÜHN¹ — ¹Experimental Condensed Matter Physics, TU Darmstadt, Germany — ²Ernst-Berl Institut für makromolekulare Chemie, TU Darmstadt, Germany

We study gold nanorods of defined length (60 nm) and diameter (20 nm) in different solvents. The nanorods are coated by a block copolymer layer (Polyisoprene-*b*-Polypropylensulfid) which enhances the miscibility of the rods in organic solvents (tetrahydrofuran, chloroform, hexane, toluene). We apply an external AC electric field up to 1000 V/mm while performing dynamic light scattering experiments (DLS) to yield in collective diffusion coefficients, relaxation times and stretching parameters. These parameters show a strong correlation with the strength of the electric field in solutions of gold nanorods in THF and chloroform. This is due to a strong dielectric response of the respective solvent which causes the nanorods to accelerate their diffusive dynamics. This effect is absent when hexane or toluene is used as solvent.

We present a detailed analysis of the dependency of the dynamical parameters on the applied electric field. The orientation of the gold nanorods depending on the electric field is investigated by small angle X-Ray scattering.

CPP 54.68 Thu 15:00 P2

maghemite nanoparticles embedded in thin block copolymer films — ●YUAN YAO¹, EZZELDIN METWALLI¹, BO SU¹, VOLKER KÖRSTGENS¹, DANIEL MOSEGUI GONZALEZ¹, LIN SONG¹, GONZALO SANTORO², STEPHAN V. ROTH², MATTHIAS OPEL³, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching — ²DESY, Notkestrasse, 85, 22603 Hamburg — ³Walther-Meissner-Institute, Walther-Meissner-Straße, 8, 85747 Garching

Maghemite nanoparticles embedded inside a polymer matrix mark a novel class of hybrid materials which have attracted high interest due to the potential for numerous applications such as sensors and high density magnetic storage devices. The control of the alignment of the maghemite nanoparticles within the polymer matrix is essential for producing well-aligned highly-oriented metal oxide-polymer nanocomposites. The alignment of maghemite nanoparticles in polystyrene-*b*-poly(*N*-isopropylacrylamide) P(S-*b*-NIPAM) diblock copolymer films is investigated. The thin hybrid films are prepared by spin coating. The structure of the resulting hybrid films is studied at different con-

centrations of maghemite nanoparticles using SEM, AFM, GISAXS and GIWAXS. The results indicate a morphological transition from lamella to hexagonal upon incorporation of maghemite nanoparticles into the diblock copolymer films. At high concentration of nanoparticles, large particles aggregates are formed on top of the polymer surface. The magnetic properties of the nanocomposite films at different temperatures are measured and compared with theoretical predictions.

CPP 54.69 Thu 15:00 P2

Whispering gallery modes in spherical copolymers — ●DANIEL BRAAM¹, KENICHI TABATA², GÜNTHER M. PRINZ¹, YOHEI YAMAMOTO², and AXEL LORKE¹ — ¹Experimentalphysik und CENIDE, Universität Duisburg-Essen — ²Faculty of Pure and Applied Sciences, University of Tsukuba, Japan

Copolymers are promising candidates for use in optoelectronic devices because of their cost efficiency and superior optical properties.

By combining polymers to π -conjugated alternating copolymers (e.g. F8TMT2 with fluorene and thiophene in the repeating units [1]), isotropic microspheres can be fabricated. By adjusting the formation parameters, their size can be tuned from some hundred nanometers to several micrometers. Laser excitation of a single sphere leads to a broad photoluminescence spectrum with superimposed narrow peaks. The number of observed peaks is dependent on the sphere diameter and they are attributed to standing waves on the inside of the sphere, known as whispering gallery modes (WGMs). The measured peak positions are in good agreement with theoretical calculations of TM- and TE-WGMs. This allows us to determine the copolymer's relative permittivity.

The investigated π -conjugated alternating polymer particles combine the properties of a dye, a dielectric and a resonator. This opens up the possibility to build photonic crystals by arranging spheres with a distinct and narrow size distribution to match and amplify certain WGMs, aiming for novel optoelectronic properties.

[1] Taeko Adachi et al., J. Am. Chem. Soc. **135**, 870 (2013)

CPP 54.70 Thu 15:00 P2

How long is the interfacial length in a nanocomposite system? — ●EVANGELOS VOYIATZIS, FLORIAN MÜLLER-PLATHE, and MICHAEL BÖHM — Eduard-Zintl-Institut für Anorganische und Physikalische Chemie and Center of Smart Interfaces, Technische Universität Darmstadt, Alarich-Weiss-Str. 4, D-64287 Darmstadt, Germany

The influence of fullerene inclusion on the structure of a polystyrene matrix as well as the spatial distribution of the atomic level stresses in the polymer and the cavity size distribution is studied by molecular dynamics simulations. The spatial deviations of the two latter quantities from their average bulk values are correlated with characteristic deviations of structural properties, such as the mass density distribution and segmental orientation of the polymer matrix. The structural properties of the polymer in the vicinity of the nanoparticle suggest the formation of two layers, a result that is in accordance with findings of previous studies. The inclusion of fullerenes enhances the stress anisotropies in their neighbourhood. This is pointed out by the magnitude of the spatial variations of both the average shear stress and the von Mises shear stress. The length of the interface formed between the fullerenes and the polystyrene matrix is estimated by monitoring the variations of the radial mass density and the radial atomic level stress distributions from their average bulk values. The two methods lead to significant differences in the estimated interfacial lengths. The values based on variations of the atomic level stresses are considerably shorter than the estimate obtained when using the variations of the mass density distribution.

CPP 54.71 Thu 15:00 P2

Work of Adhesion between Metals and Polymers on a Macro- and Microscopic Scale — ●MARIEKE FÜLLBRANDT, DIKRAN KESAL, and REGINE VON KLITZING — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Strasse des 17. Juni 124, 10623 Berlin

Polymer/metal hybrids are of high interest for example in lightweight constructions used in the automotive industry. They combine a high functional integration with a lower weight compared to pure metal parts. The joining of these dissimilar materials without using additional material is a central challenge. A fundamental understanding about the adhesion mechanisms at the polymer/metal interface is inevitable.

In this contribution the work of adhesion between different metal/polymer systems relevant for industrial applications is studied

by atomic force microscopy (AFM) and contact angle (CA) measurements. AFM is used for the determination of the pull-off force between a metal substrate and a polymeric microsphere. Measurements are conducted in a dry nitrogen atmosphere at 30 °C. The measured adhesion forces are analyzed using theoretical models of contact mechanics. Different models are discussed and the effect of roughness is considered. With CA measurements the surface energy of the solids is determined. From that the interfacial energy between a given metal/polymer system can be determined and further be related to the work of adhesion. Results from AFM and CA measurements are compared and possible adhesion phenomena are discussed.

CPP 54.72 Thu 15:00 P2

Structure-Property relationships of Nanocomposites Based on Epoxy and Layered Double Hydroxides — ●JING LENG¹, FRANZISKA EMMERLING¹, DE-YI WANG^{2,3}, and ANDREAS SCHÖNHALS¹ — ¹BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany — ²IMDEA Materials Institute, 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

Two kinds of organically modified MgAl Layered Double Hydroxides (MgAl-LDH) were synthesized and reaction blended with an epoxy system (EP) to obtain polymerbased nanocomposites. The organic modification of the MgAl-LDHs were by sodium dodecylbenzene sulfonate (SDBS) modified and own synthesized SACC. The two kinds of nanocomposites were investigated by a combination of differential scanning calorimetry (DSC), small- and wide-angle X-ray scattering (SAXS and WAXS), and broadband dielectric spectroscopy (BDS) in dependence of the concentration of the nanofiller. The differences observed for the both kinds of nanoparticles are discussed in detail.

CPP 54.73 Thu 15:00 P2

Interactions between capped gold nanocrystals in vacuum: presence of three-body effects — ●NADEZDA GRIBOVA¹, GERNOT BAUER¹, CHRISTIAN HOLM², and JOACHIM GROSS¹ — ¹ITT, University of Stuttgart, Stuttgart, Germany — ²ICP, University of Stuttgart, Stuttgart, Germany

Self-assembly of capped nanocrystals became an active topic during the last years. Nanocrystals are currently used in many areas of engineering and life sciences or medicine. However, a full understanding of their mechanical and thermodynamical stability is still lacking. Nanocrystals are usually capped with some organic ligands, which prevent aggregation. These capping molecules play an important role in the self-assembly of the nanoparticles – the ratio between the ligand length and the diameter of the nanocrystal core determines the structure of the superlattice in which nanoparticles assemble.

In this study, we report the potential of mean force between gold nanocrystals capped with alkythiols. We propose a simple but accurate temperature-scaling of this effective pair potential, based on a perturbation theory. Schapotschnikow and Vlught [1] have shown that effective three-body interactions exist between capped nanocrystals. We analyze the dependence of the 3-body contribution on different ligand lengths and core sizes and show that the 3-body potential does not significantly depend on the temperature. We also propose a three-body potential that scales with the repulsive part of the effective pair potential.

[1] P. Schapotschnikow et al., Nano. Lett. **8**, 2930, (2008)

CPP 54.74 Thu 15:00 P2

The effect of electric fields on CdSe-nanocrystals — ●ROBERT NIEMÖLLER, DANIEL BRAAM, GÜNTHER M. PRINZ, MARTIN GELLER, and AXEL LORKE — Experimentalphysik und CENIDE, Universität Duisburg-Essen

Using a micro-photoluminescence (μ -PL) setup, we investigate field-induced spectral changes in the emission of CdSe/ZnS nanocrystals, pumped with a Nd:YVO₃ laser. We embed the nanocrystals between two layers of polymethylmethacrylat (PMMA) and place them inside a capacitor-like structure consisting of a doped silicon substrate and thin transparent metal electrodes. Thus, we are able to subject the crystals to a tunable electric field and record their PL simultaneously. Small agglomerates of crystals show different behavior in their PL when a voltage is applied, depending on the substrates used. The samples with p-doped substrates show a shift in their peak energy, which is proportional to the square of the applied voltage, caused by the quantum-confined Stark effect. From this dependency we can extract the polarizability of the nanocrystals which is in good agreement

with values measured by other groups on a different sample structure. However, the samples prepared on n-doped substrates only show a shift when a negative voltage is applied to the metal electrode, leading to an asymmetric Stark shift. When cooled down to approximately 15 K, the structures on p-doped substrates exhibit a similar asymmetric dependence of the PL energy on the applied voltage.

CPP 54.75 Thu 15:00 P2

Unexpected low-frequency dynamics in DGEBA/SiO₂ — ●RICK DANNERT¹, PATRICK ELENS¹, MATTHIEU THOMASSEY², JÖRG BALLER¹, and ROLAND SANCTUARY¹ — ¹Laboratory for the Physics of Advanced Materials, University of Luxembourg — ²G2IP / ICPEES CNRS UMR 7515 - ECPM / University of Strasbourg (France)

We investigate the complex rheological behaviour of nanocomposites based on low molecular weight epoxy resins. The resin consists of DGEBA (diglycidylether of Bisphenol-A) with different degrees of polymerization (monomers, dimers, trimers). The nanoparticles (diameter: 25 nm) consist of silica coated with a thin silane layer to achieve a good dispersion. In order to investigate the relaxation behaviour of the complex shear moduli, we exploit dynamic rheology at temperatures higher than the thermal glass transition temperature (258K). Measurements of the pure viscoelastic DGEBA system show powerlaw behaviour. The dynamic glass transition is shifted to lower frequencies by adding nanoparticles. In addition to the alpha process, the shear moduli show unexpected relaxations at much lower frequencies. These low-frequency relaxations are systematically investigated for different nanoparticle concentrations and by changing the relaxation dynamics of the matrix molecules. The latter is done by specifically modifying the length of the matrix molecules, e.g. by using dimers instead of monomers.

CPP 54.76 Thu 15:00 P2

Characterization of the electronic and magnetic structure of multifunctional NaREF₄ (RE = rare earth) core-shell nanoparticles — ●LILLI SCHNEIDER¹, THORBEN RINKEL², ARTUR CHROBAK³, MARKUS HAASE², and KARSTEN KÜPPER¹ — ¹Physics Department, University of Osnabrück, Germany — ²Institute of Chemistry, University of Osnabrück, Germany — ³Institute of Physics, University of Silesia, Poland

Rare earth (RE) based nanoparticles of type NaREF₄ have attracted lot of attention in the last few years due to their upconverting luminescence. Here, we want to concentrate on electronic and magnetic properties of NaREF₄/NaGdF₄ nanocrystals, since the magnetic behaviour of these fluorescent nanoparticles are of utmost importance from fundamental and applicative point of view as well. Hexagonal β -phase nanocrystals (3-22 nm) were prepared and characterized by X-ray powder diffraction (XRD) and transmission electron microscopy (TEM).

A detailed study of the electronic structure and magnetic coupling phenomena of the different core-shell nanoparticles is performed using X-ray photoelectron spectroscopy (XPS), magnetometry (SQUID) and X-ray magnetic circular dichroism (XMCD). First SQUID measurements of NaEuF₄/NaGdF₄ core-shell nanoparticles show butterfly shaped hysteresis loops at low temperature (2 K) in contrast to superparamagnetic behaviour observed for the corresponding "pure" NaEuF₄ and NaGdF₄ nanoparticles.

CPP 54.77 Thu 15:00 P2

Role of geometric parameters on nanoparticle-polymer brush composite systems — ●MURIEL ROVIRA ESTEVA, STEFAN WELLERT, and REGINE VON KLITZING — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Institut für Chemie, Technische Universität Berlin, Straße des 17. Juni 124, 10623 Berlin, Germany

Polymer brushes are polymers tethered to a surface or interface by one end, which at sufficiently high grafting densities show a stretched conformation away from the surface. Many of its applications involve interaction with particles of some kind, so understanding the interactions between nanoparticle and polymer brushes is of great importance.

A number of parameters may play a significant role on the structure as well as the dynamics of these systems (particle characteristics, brush morphology, polymer-nanoparticle interaction, solvent quality, etc.), but the extremely small sample volume and complexity of the system have rendered the experimental investigation of their influence a challenging task. Poly(2-(dimethylamino)ethyl methacrylate) (PDMAEMA) brushes with embedded gold nanoparticles have been used as model systems in this work to explore the effect of the various parameters on the composites and obtain a global picture of their

behaviour, particularly in their swollen state.

CPP 54.78 Thu 15:00 P2

Plasmonic nanoparticle assemblies with controllable plasmon resonance coupling — ●TOBIAS HONOLD¹, MAREEN MÜLLER², ANDREAS FERY², and MATTHIAS KARG¹ — ¹Physical Chemistry I, University of Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — ²Physical Chemistry II, University of Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany

Surface plasmon resonances are collective oscillations of the electron gas at a metal surface which can be excited by electromagnetic radiation. These resonances become localized when the size of the metal object is reduced down to the nanoscale. The energy of this localized surface plasmon resonance (LSPR) depends strongly on the particle size, shape, the dielectric environment and on the metal itself. In addition, LSPRs are sensitive to the inter-particle distance. When two plasmonic nanoparticles approach each other coupling of the resonances occurs and the optical properties of the system can change significantly. In this contribution we show how we make use of this distance dependent coupling behavior in order to create plasmonic surfaces with tailored optical properties. In our approach we coat the plasmonic nanoparticles with polymer shells which then act as a steric spacer during particle assembly. These core-shell particles can nicely be assembled to form hexagonal close-packed monolayer or more complex structures such as linear assemblies realized through wrinkle-assisted assembly. The inter-particle separation is controlled by the thickness of the polymer shell and hence plasmon resonance coupling becomes controllable

CPP 54.79 Thu 15:00 P2

Dendronized polymers replicated with graphene and graphene oxide — ●SIMONE DELL'ELCE¹, VITALIJ SCENEV¹, BAOZHONG ZHANG², NIKOLAI SEVERIN¹, DIETER SCHLÜTER², and JÜRGEN P. RABE¹ — ¹Department of Physics, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — ²Laboratory of Polymer Chemistry, Department of Materials, ETH Zürich, Wolfgang Pauli Strasse 10, HCI J541, 8093 Zürich, Switzerland

Graphene has been demonstrated to be highly bendable and stretchable to follow the topography of a solid surface with the precision down to single macromolecules (N. Severin et al., Nano Lett. 2011, 11, 2436). The question remains, in how far the locally strained graphene may have an impact on the conformation of the replicated macromolecules. Dendronized polymers (denpols) consist of a linear backbone surrounded by a dense cladding of structurally regular dendritic branches (dendrons), anchored to each repeating unit. Variation of the dendron generation allows to tune the properties of the denpols. We deposited denpols on an atomically flat mica substrate and covered them with either graphene or graphene oxide (GO) layers. Scanning force microscopy images reveal that the heights of the denpol replicas in GO match the heights of uncovered molecules. The heights of higher generation denpol replicas in graphene are substantially smaller as compared with the heights of the uncovered macromolecules. This may be attributed to graphene being stiffer than GO and more strongly interacting with the substrate, collapsing thereby to some extent the structure of the high generation denpols

CPP 54.80 Thu 15:00 P2

Controlled drug release using nanodiamonds as drug carriers — ●TRAN MINH VU, ANDREA KURZ, ANNA ERMAKOVA, GOUTAM PRAMANIK, BORIS NAYDENOV, YUZHOU WU, TANJA WEIL, and FEDOR JELEZKO — University Ulm

We investigated the drug release of nanodiamond- Doxorubicin (ND-DOX) complexes in different pH. DOX is a chemotherapeutic against cancer cells, e.g. mammary or liver tumors. Using untreated DOX in order to kill cancer cells has two main problems: DOX also affects healthy cells and cancer cells can be resistant through drug efflux [1]. These problems can be overcome by using ND-DOX complexes [1]. Nanodiamonds are non-toxic [2], can move through membrane cells [2] and their surface can be functionalized making them able for drug delivery. Cancer cells have a lower pH environment compared to healthy cells, therefore we did a pH-sensitive experiment. We prepared a sample of ND-DOX in a solution at pH 7. With a standard confocal setup we performed fluorescence correlation spectroscopy (FCS) and determined the hydrodynamic radius r . We observed that by changing the pH of the ND-DOX solution from 7 to 5 the radius $r=130$ nm at pH=7 decreased to $r=6$ nm at pH=5. The fluorescence signal came from DOX (our NDs are non-fluorescent) thus indicated DOX release

from the bigger ND-DOX complex. These measurements can be done time- dependent, respectively pH dependent leading to drug release time and the pH value which triggers the release. [1] Chow et al., *Sci. Transl. Med.* 3, 73ra21 [2] Chi-Cheng Fu et al., *PNAS* 104 (3) 727-732

CPP 54.81 Thu 15:00 P2

Resonance Energy Transfer Between Nanotubular J-Aggregates and Quantum Dots — •YAN QIAO¹, FRANK POLZER¹, SERGEI KÜHN², SEBASTIAN FRIEDE², STEFAN KIRSTEIN¹, and JÜRGEN RABE¹ — ¹Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — ²Max-Born-Institut für Nicht-lineare Optik und Kurzzeitspektroskopie im Forschungsverbund Berlin e.V., Max-Born-Straße 2 A, 12489 Berlin, Germany

Resonance coupling between distinct excitons in organic / inorganic hybrid materials has become a promising approach towards the design of novel nano-structured opto-electronic devices [1,2]. Herein we report on the construction of colloidal nanohybrids built in aqueous solution from tubular J-aggregates of amphiphilic cyanine dyes and semi conducting quantum dots (QDs) of CdTe. QDs of different size were attached to the surface of the J-aggregates by electrostatic self-assembly. The close proximity between J-aggregates and QDs enables strong coupling between the dissimilar excitons with high energy transfer efficiencies. The direction of energy transfer is selected by the size of the QDs. FRET efficiency of 92% is achieved for transfer from QDs to the J-aggregates. For the opposite direction the J-aggregates act as light harvesting antennas and increase the effective absorption of the QDs by a factor of ten.

[1] B. J. Walker, V. Bulović, M. G. Bawendi, *Nano Lett.* 2010, 10, 3995.

[2] Q. Zhang, T. Atay, J. R. Tischler, M. S. Bradley, V. Bulović, A. V. Nurmikko, *Nat. Nanotechnol.* 2007, 2, 555.

CPP 54.82 Thu 15:00 P2

Long-term time-resolved photoluminescence studies of novel Ruthenocenyldecorated Sn/S cluster — •NILS ROSEMAN¹, ELIZA LEUSMANN², MONA WAGNER², STEFANIE DEHNEN², and SANGAM CHATTERJEE¹ — ¹Fachbereich Physik Philipps-Universität Marburg, Marburg, Germany — ²Fachbereich Chemie Philipps-Universität Marburg, Marburg, Germany

The use of ruthenium complexes opens a variety of applications, such as dye-sensitized solar cells and chromophores[1,2]. Single-crystals of novel core shell clusters with ruthenocene-ligand and inorganic Sn4S6 core were grown. As such crystals are known to be rather sensitive to irradiation; we perform long-term low-density photoluminescence measurements. To address individual single crystals, these are performed using a streak-camera setup with high spatial resolution in the μm range. This way, the spectral information and ultra-fast carrier dynamics are investigated. Combining these information gives rise to any optical induced changes of the crystals.

[1] *Angew. Chem.* 123, 10870-10873, (2011)

[2] *Inorg. Chem.* 50, 5494-5508, (2011)

CPP 54.83 Thu 15:00 P2

Characterization of carbon nanotube containing polymer membranes — •TÖNJES KOSCHINE¹, KLAUS RÄTZKE¹, VOLKER ABETZ², THOMAS EMMER², MUNTAIM MUNIR KHAN², VOLKAN FILIZ², LUCA RAVELLI³, WERNER EGGER³, and FRANZ FAUPEL¹ — ¹CAU Kiel, Technische Fakultät, Institut für Materialwissenschaft, Kiel — ²Helmholtz-Zentrum Geesthacht, Zentrum für Material- und Küstenforschung GmbH, Geesthacht — ³Universität der Bundeswehr München, Fakultät für Luft- und Raumfahrttechnik, Neubiberg

Polymeric membranes are widely used for gas separation, where free volume is a key property for characterization. High free volume membranes, for instance PIM-1, are suitable candidates. Positron annihilation lifetime spectroscopy (PALS) is a well-established method for free volume measurements and has already been applied to these polymers [1]. In membrane applications the polymers have to be prepared as thin films and undergo aging, usually related to reduced free volume and resulting in reduced permeability. This has already been characterized by PALS [2]. In the present investigation we characterized thin films of PIM-1 and PIM-1 with 2 wt% of functionalized multiwall carbon nanotubes (f-MWCNT) on porous support (PAN). The typical thickness of the films was about 700 nm and therefore a moderated beam for positron lifetime analysis was used. All samples were measured in the as prepared state and after 300 days of aging. Results show, that incorporation of f-MWCNT into PIM results in reduced aging.

[1] R. Lima de Miranda et al., *Phys. Stat. Sol. RRL* 1(5), 2007, 190ff

[2] S. Harms et al., *Journal of Adhesion* 88, 2012, 608-619

CPP 54.84 Thu 15:00 P2

Chain conformation of poly(butylene oxide) silica nanocomposites — •ADRIAN HAMM, WIM PYCKHOUT-HINTZEN, ANDREAS WISCHNEWSKI, JÜRGEN ALLGAIER, and DIETER RICHTER — Jülich Centre for Neutron Science JCNS and Institute for Complex Systems ICS, Jülich, Deutschland

Poly(butylene oxide) silica mixtures have proven to be a nanocomposite model system with many desirable features. As poly(butylene oxide) does not crystallize this opens up the possibility to investigate its behaviour with many different methods over a very broad temperature range. After preliminary small angle x-ray scattering experiments to prove good particle dispersion we used rheology and boradband dielectric spectroscopy experiments to gather information about the changes in sample behaviour that can be introduced by adding silica nanoparticles. As a next step we wanted to gain more microscopic insight and performed small angle neutron scattering experiments on our samples. We now want to present first results of these recent experiments on poly(butylene oxide) silica nanocomposites and show what we learned about the change in chain conformation introduced by the nanoparticles.

CPP 54.85 Thu 15:00 P2

Upconversion Quantum Yields of Rare Earth Doped Nanoparticles dependent on dopant concentration — •MARTIN KAISER¹, WÜRTH CHRISTIAN¹, HYPÄNEN IKO², EMILIA PALO², SOUKKA TERO², and RESCH-GENGER UTE¹ — ¹BAM Bundesanstalt für Material- forschung und -prüfung, Richard-Willstätter-Str. 11, 12489 Berlin — ²Department of Biotechnology, University of Turku, Tykistökatu 6A, FI-20520 Turku, Finland

Hexagonal $\beta\text{-NaYF}_4$ doped with Er^{3+} and Yb^{3+} is currently the most efficient up-conversion (UC) or also called 'Anti-Stokes' phosphor which converts near-infrared (NIR) to green light. The design of efficient nm-sized UC particles requires reliable spectroscopic tools for the characterization of the signal-relevant optical properties of these materials like the up-conversion quantum yield (UC QY), which equals the ratio of high energy photons emitted to low energy photons absorbed. We present here a custom-designed integration sphere setup equipped with a high-power 980 nm-laser diode for spectrally resolved and power density-dependent measurements of UC QY. Power dependent UC QY and luminescence lifetime measurements of nm-sized $\beta\text{-NaYF}_4\text{:Er}^{3+}$, Yb^{3+} with different dopant concentrations will be discussed.

CPP 55: Mitgliederversammlung des Fachverbandes CPP

Alle Mitglieder des Fachverbandes CPP sind herzlich eingeladen.

Time: Thursday 19:00–20:00

Location: ZEU 222

Mitgliederversammlung

CPP 56: Colloids and Complex Liquids IV

Stabilization

Time: Friday 9:30–10:30

Location: ZEU 260

CPP 56.1 Fri 9:30 ZEU 260

Form fluctuations of polymer loaded spherical microemulsions — ●BJÖRN KUTTICH¹, PETER FALUS², ISABELLE GRILLO², and BERND STÜHN¹ — ¹Experimental Condensed Matter Physics, TU Darmstadt, Germany — ²Institut Laue-Langevin, Grenoble, France

Spherical microemulsions with the anionic surfactant AOT are well suited as model system with a soft confining geometry. Their structural and dynamical properties are already intensively studied by various scattering methods and the droplet radius, determining the confinement size, can easily be tuned by the precise composition of the microemulsion. A first approach of applying this confinement to complex molecules is the investigation of small simple polymers like PEO in the microemulsions droplets. Besides the influences of the polymer on the phase diagram of the microemulsion, changes in the droplet dynamics are of great interest.

Neutron spin echo spectroscopy is a unique method to investigate the fluctuations of the microemulsions surfactant shell and how they are influenced by the presence of polymers. Droplet phase Water/AOT/Octane microemulsions with different radii and polymer content were investigated at the ILL at IN15, their droplet structure was secured by SANS on D11. Measuring the relaxation rate of the fluctuations the bending modulus of the shell can be determined by hydrodynamic calculations and a softening of the shell with addition of polymer is observed. This finding is complemented by percolation temperature measurements by dielectric spectroscopy.

CPP 56.2 Fri 9:45 ZEU 260

Rationalizing Polymer Swelling and Collapse under Attractive Cosolvent Conditions — ●JAN HEYDA¹ and JOACHIM DZUBIELLA^{1,2} — ¹Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, Hahn-Meitner Platz 1, 14109 Berlin, Germany — ²Department of Physics, Humboldt-University Berlin, Newtonstr. 15, 12489 Berlin, Germany

The collapse and swelling behavior of a generic homopolymer is studied using implicit-solvent, explicit-cosolvent Langevin dynamics computer simulations for varying interaction strengths. Maximal swelling is observed if both monomer-monomer and monomer-cosolute interactions are weakly attractive. In the most swollen state the cosolute density inside the coil is remarkably bulk-like and homogenous. Highly attractive monomer-cosolute interactions, induce a chain collapse with considerably enhanced cosolute density within the globule, in strong contrast to the collapse in purely repulsive cosolvents. Thus, similarly appearing collapsed states may result from very different mechanisms with distinct final structural and thermodynamics. Two theoretical models, one based on an effective one-component description, and a fully two-component Flory – de Gennes like model, are in accord with simulation findings. In particular, the polymer collapse in highly attractive cosolvents driven by crosslinking-like bridging effects is reproduced. Next, swelling is predicted only for not too short-ranged interactions. Our findings has implications for cosolute effect on conformations of biomolecules, in particular for highly attractive cosolutes, such as urea, GdmCl, NaI, or NaClO₄ near peptide-like moieties.

CPP 56.3 Fri 10:00 ZEU 260

Conosolvency in P(S-*b*-NIPAM) diblock copolymers - a time-resolved SANS study of the aggregation process — ●KONSTANTINOS KYRIAKOS¹, MARTINE PHILIPP¹, JOSEPH ADELSBERGER¹, SEBASTIAN JAKSCH¹, ISABELLE GRILLO², ANNA MIASNIKOVA³, ANDRÉ LASCHEWSKY³, PETER MÜLLER-BUSCHBAUM¹, and CHRISTINE M. PAPADAKIS¹ — ¹TU München, Physik-Department, Garching — ²Institut Laue-Langevin, Grenoble, France — ³Universität Potsdam, Institut für Chemie, Potsdam-Golm

In mixtures of water and methanol, the thermoresponsive poly(N-isopropylacrylamide) (PNIPAM) exhibits the conosolvency effect, i.e. an enhanced tendency for phase separation at certain solvent compositions. The amount of consolvent may have a severe effect on the pathway of the collapse of the PNIPAM chain and the subsequent aggregation into mesoglobules, in line with previous experiments where aqueous solutions of PNIPAM were heated through the cloud point.

We report here on time-resolved small-angle neutron scattering experiments during the rapid addition of methanol to aqueous solutions of P(S-*b*-NIPAM). These block copolymers form core-shell micelles with a thermoresponsive shell. Small aggregates are formed very rapidly and growth with time reaching a certain size. The kinetics of this aggregation path depends on the amount of methanol. The observed growth process can be adequately described by the diffusion-limited coalescence model, and proceeds in a different way than previously observed in temperature jumps across the cloud point [1].

[1] Adelsberger, J. et al. *SoftMatter* **9**, 1685 (2013)

CPP 56.4 Fri 10:15 ZEU 260

Dehydration behavior of phase separating PNIPAM solutions — ●MARTINE PHILIPP¹, KONSTANTINOS KYRIAKOS¹, LUCA SILVI^{1,2}, WIEBKE LOHSTROH^{1,2}, WINFRIED PETRY^{1,2}, JAN K. KRÜGER³, CHRISTINE M. PAPADAKIS¹, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien/FG Physik weicher Materie, Garching, Germany — ²TU München, MLZ, Garching, Germany — ³Université du Luxembourg, LPM, Luxembourg, Luxembourg

A structural instability leads to the collapse and aggregation of poly(N-isopropyl acrylamide) (PNIPAM) in aqueous environment at an LCST-type demixing transition. This transition is provoked by the interplay of H-bond and hydrophobic interactions between PNIPAM and water. The cooperative dehydration of PNIPAM plays a key role for the genesis of the PNIPAM-rich globules. Using quasi-elastic neutron scattering, we elucidate for the first time the partial dehydration process of PNIPAM in a concentrated solution. As the hydration number decreases from 8 to 2 during phase separation, the PNIPAM-rich globules contain at most 75 mass% PNIPAM. First insights into the relationship between the molecular dehydration process and the ensuing macroscopic changes of order parameter susceptibilities are presented for dilute to concentrated PNIPAM solutions, studying the volume expansion coefficient and compressibility [1,2].

[1] M. Philipp et al., *Soft Matter* **8**, 11387 (2012)

[2] M. Philipp et al., *Soft Matter* **9**, 5034 (2013)

CPP 57: Physics of Food

Time: Friday 10:45–12:15

Location: ZEU 260

Invited Talk

CPP 57.1 Fri 10:45 ZEU 260

Crystallization in Food — •HANS JÖRG LIMBACH¹, KONSTANTIN KOSCHKE², and DAVIDE DONADIO² — ¹Nestlé Research Center, Lausanne, Switzerland — ²MPI for Polymer Research, Mainz, Germany

The paper will start with a short introduction covering various aspects of the role of crystallization in food products like ice cream, frozen meals, chocolate and beverage powders.

The main part will focus on recent work on the thermodynamics of freezing point depression in solutions that has been carried out in collaboration with the Max-Planck-Institute for Polymer Research. We will show how the freezing point depression changes as a function of the similarity between the solvent and the solute molecules. The influence of the solute molecules on the liquid structure of the solvent will be discussed. In addition a suitable thermostat to study the kinetic limit of crystal growth rates in a model system will be presented. The work is based on molecular dynamic simulations using binary Lennard-Jones model systems.

As the last part of the contribution a small number of open problems related to crystallization in food will be put forward for further discussion.

CPP 57.2 Fri 11:15 ZEU 260

Molecular migration in multicomponent food products — •SVENJA REINKE¹, STEPHAN V. ROTH², GONZALO SANTORO², JOHN RASBURN³, STEFAN PALZER⁴, and STEFAN HEINRICH¹ — ¹Hamburg University of Technology, Hamburg, Germany — ²HASYLAB/DESY, Hamburg, Germany — ³Nestlé PTC, York, United Kingdom — ⁴Nestlé SA, Vevey, Switzerland

Controlling the molecular migration of molecules through complex food products is of high interest in food technology: This process is leading to major quality issues such as fat blooming of chocolate resulting in large sales losses for the food industry.

In general, the complex, multicomponent food products investigated consist of particles surrounded by a continuous lipid matrix. The molecules could migrate through the continuous matrix phase, through the phase composed by the embedded particles or via the interface of matrix and particles. However, this mechanism of migration through multicomponent materials is still not well understood. Therefore, the microstructure of the multicomponent material is analyzed and visualization of the migration path within the matrix is intended. Using microbeam small-angle X-ray scattering (μ SAXS) at the MiNaXS/P03 beamline at DESY we investigated oil migration through multicomponent products. Thereby, the effect of different oils and their possible influence on structural changes was analyzed. To get further insight into possible pathways, the wetting properties of the hydrophobic and hydrophilic components are analyzed. We present a model to describe the migration on a molecular level based on molecular simulations.

CPP 57.3 Fri 11:30 ZEU 260

Understanding protein denaturation, water loss and texture during sous-vide cooking of pork filet — •BIRGITTA ZIELBAUER¹, BENJAMIN VIEZENS^{1,2}, JOHANNES FRANZ¹, and THOMAS VILGIS¹ — ¹Max-Planck-Institut für Polymerforschung, Mainz, Germany — ²Beuth Hochschule für Technik, Berlin, Germany

Meat is a highly complex natural product, comprising a wide range of different proteins assembled into complex structures, which form the muscle fibers as well as connective tissue. Besides taste, the main factor influencing the sensory perception of a cooked piece of meat is its texture. This depends - besides of intrinsic factors such as animal type and age or muscle type, which determine the properties of the raw product - crucially on protein denaturation stages and related water content of the final product. Sous-vide cooking offers the possibility to precisely control those factors by choosing appropriate time-temperature combinations and thus selectively denature specific proteins while keeping others intact.

The denaturation kinetics of the meat proteins (such as myosin, collagen, actin, and sarcoplasmic globular proteins) can be followed by differential scanning calorimetry (DSC). For longer times, proteins denature below their denaturation temperature obtained from DSC measurements, which can be roughly explained by a statistical and kinetic model. These results are related to water content and textural characteristics of the samples.

Invited Talk

CPP 57.4 Fri 11:45 ZEU 260

Soft Matter Multi-Scale Food Physics - Texture, Taste and Aroma — •THOMAS VILGIS — Max-Planck-Institut für Polymerforschung

The common point of the large variety of raw, cooked, and processed foods is that they are multi-component materials which consist at least of proteins, carbohydrates, fat and water. Their concentration ratios define most of the structural and textural properties of the foods. Given the different solubility of these components in the basic solvents water and fat, it becomes clear that many physical properties, such as structure and texture are determined by a large number of competing interactions between these different components. The conformation and dynamics of water soluble long carbohydrates and partially water soluble native or denatured proteins determine together with the water content the textural properties of foods. In addition, local short range interactions of these macromolecules with comparatively small ions (salts), polar molecules (water, low molecular weight sugars) and amphiphilic molecules (emulsifiers) have a strong influence on macroscopic properties, such as texture and mouth feel as it is demonstrated with simple model systems such as multi-component gels with special rheological properties and resulting physics based sensory qualities.

CPP 58: Polymer Dynamics II

Time: Friday 9:30–11:15

Location: ZEU 114

Invited Talk

CPP 58.1 Fri 9:30 ZEU 114

Probe Rheology with Neutron Scattering — •WIM PYCKHOUT-HINTZEN — Jülich Centre for Neutron Science (JCNS-1) and Institute for Complex Systems (ICS-1), Forschungszentrum Jülich, Germany

An improved understanding of the nonlinear rheology of complex mixtures of polymers with different architectures for e.g. processing applications is a formidable task and one of today's challenges in polymer science. Therefore, blends of model branched and linear polymers with strongly disperse time scales were investigated with time-dependent small angle neutron scattering after a fast uniaxial step strain and quenched after different relaxation times. A hyperbranched structure of second generation, dilutely dispersed in linear homopolymer matrices of different length acted thereby like sensitive probes for structurally, not yet firmly established features of the tube model for bi-disperse melts. We show that the equilibration time of the linear matrix determines the size of the fluctuations that the outer and inner arms of the branched probe experience. Within a random phase approximation treatment, accounting for different degrees of freedom in-

herent to the broad time scales and the hierarchical relaxation scheme, the observed loss of anisotropy with time is described in terms of two parameters only, namely the tube diameter and the fraction of relaxed arms of the minority component. The scattering data reveal the underlying mechanisms, which cannot be extracted from but determine the macroscopic flow properties. This information is a prerequisite to quantify the nonlinear viscoelasticity for the strategic blending of mixed architectural systems.

CPP 58.2 Fri 10:00 ZEU 114

Network structure and entanglement effects in saturated and unsaturated acrylonitrile elastomers — •PATRICK STRATMANN^{1,2}, FRANK FLECK^{1,2}, and MANFRED KLÜPPEL^{1,2} — ¹Deutsches Institut für Kautschuktechnologie e.V. — ²Eupener Straße 33, 30519 Hannover

Differently cross-linked, saturated and unsaturated acrylonitrile elastomers (HNBR, NBR) are investigated regarding their entanglement contributions in uniaxial stress strain measurements. Our main focus

lies on the assessment of the *non affine* tube model and *slip tube* model in analysing the mechanical data, whereby the influence of entanglement contributions on the fitted topological constraint modulus and crosslink modulus are considered. Conclusions on the validity or invalidity of specific tube theories cannot be drawn without careful consideration of the network microstructure, which determines the entanglement density. Rheological investigations of the viscoelastic response show a difference in the plateau modulus between the nitrile rubber and the hydrogen nitrile rubber due to different entanglement densities. The analysis of the stress strain and rheological data are compared. The *non affine* tube model, which has been extended to consider finite chain extensibility, delivers excellent fits to the measured stress strain data and fair correlations with the estimated entanglement density from the measured plateau modulus.

CPP 58.3 Fri 10:15 ZEU 114

Local Dielectric Spectroscopy to detect Dynamic Heterogeneity and Phase Separation Kinetics in Miscible Poly(vinyl acetate)/Poly(ethylene oxide) Blends — TOMAS P. CORRALES¹, DAVID LAROZE², GEORGE ZARDALIDIS³, GEORGE FLOUDAS³, HANS-JÜRGEN BUTT¹ und •MICHAEL KAPPL¹ — ¹MPI for Polymer Research, Mainz, Germany — ²Instituto de Alta Investigación, Universidad de Tarapacá, Arica, Chile — ³Department of Physics, University of Ioannina, Ioannina, Greece

We employed atomic force microscopy based local dielectric spectroscopy (LDS) to analyze the miscible blend composed of poly(vinyl acetate) (PVAc) and poly(ethylene oxide) (PEO). The two homopolymers have very different relaxation times and glass temperatures, which give rise to dynamic heterogeneity in their blends. The aim was to study the dynamic heterogeneity in films as a function of the film thickness. Measurements of the local blend composition at the nanoscale show that LDS is indeed sensitive to the dynamic heterogeneity. In thin films, phase segregation of the homopolymers occurs due to heterogeneous nucleation and crystallization of PEO. We were able to follow the kinetics of phase demixing by detecting the change in local composition of blends including depletion zones of PEO in the PVAc/PEO blend around the PEO crystals via LDS spectra. These results open new possibilities for studying surface segregation in polymer blends, local variation in polymer concentration, and interdiffusion at polymer-polymer interfaces as a function of annealing temperature with LDS.

CPP 58.4 Fri 10:30 ZEU 114

Structure and Dynamics of Supramolecular Polymers by Neutron Scattering — •ANA R. BRÁS, MARGARITA KRUTYEVA, CLAAS HÖVELMANN, WIEBKE ANTONIUS, JÜRGEN ALLGAIER, WIM PYCKHOUT-HINTZEN, ANDREAS WISCHNEWSKI, and DIETER RICHTER — Forschungszentrum Jülich, JCNS-1/ICS-1, D52425 Jülich, Germany

Supramolecular polymers allow a specific tailoring of polymer properties. A recent addition are self-healing polymers, displaying hydrogen-bonding interaction. The conformation and dynamics of self-healing model telechelic polymers, consisting of polypropylene glycol (PPG) end-functionalized with hydrogen-bonded associating groups was investigated by means of Small Angle Neutron Scattering (SANS) and Neutron Spin Echo (NSE) spectroscopy. SANS in deuterated toluene confirmed a linear conformation of the studied system. The scattering data were examined using an RPA model approach, usually ap-

plied to pure polymer systems. It revealed a reasonable description of the SANS data. More, it underlined the importance of chemical interactions between the components. NSE performed under the same conditions, revealed that the dynamics slowed down upon association. The NSE data were analyzed in terms of a modified Zimm model for polymer dynamics in solution taking into account an additional internal friction originating from the hydrogen-bonded groups. It was unambiguously proven that dynamic neutron scattering is probing the association by H-bonding mechanism. For the first time such an association process in solution was observed by quasielastic neutron scattering. Supported by DFG-SPP1568.

CPP 58.5 Fri 10:45 ZEU 114

Passive and active microrheology of a polymer melt studied by molecular dynamics simulation — •ANJA KUHNHOLD and WOLFGANG PAUL — Institute of Physics, Martin-Luther-University Halle-Wittenberg

The rheological behaviour of a material is determined by the relaxation of its stress autocorrelation [1]. In simulation studies the stress tensor can explicitly be calculated and serves as a reference for the microrheological results, that are based on the behaviour of suspended particles [2]. The system under study is the well established bead-spring polymer melt model [3] including one or two nanoscopic particles.

Passive microrheology yields linear response properties of the polymer melt by looking at the thermal motion of the nanoparticles. From the mean squared displacement of the nanoparticles the complex modulus $G^*(\omega)$ of the melt is determined by using a generalized Stokes-Einstein equation. The results are in very good agreement to the stress autocorrelation results. With regard to hydrodynamic effects, a more complete form of the analysis is discussed [4].

[1] M. Vladkov, J.-L. Barrat, *Macromol. Theory Simul.* **15**, 252 (2006).

[2] T. G. Mason, *Rheol. Acta* **39**, 371 (2000).

[3] C. Bennemann et al., *Phys. Rev. E* **57**, 843 (1998).

[4] A. Erbas et al., *Eur. Phys. J. E* **32**, 147 (2012).

CPP 58.6 Fri 11:00 ZEU 114

A Highly Parallelizable Monte Carlo Method For Simulating Polymeric Systems — •CHRISTOPH JENTZSCH¹, RON DOCKHORN¹, MARCO WERNER¹, and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden, Germany — ²TU-Dresden, Institut für theoretische Physik, Germany

We show a new variant of the Bond Fluctuation Model (BFM), a coarse grained algorithm to simulate polymer systems. Our model is based on a bcc lattice instead of a simple cubic lattice used for the original BFM. This leads to a modified set of bond vectors, as well as larger moves. The algorithm allows for a very efficient parallelization which is based in subdividing the bcc lattice in two disjunct sublattices. By implementing our algorithm on a consumer graphic card, we gain an upspeed of about two orders of magnitude as compared to the CPU-implementation. We compare our model with the original BFM for dense polymer melts with respect to static and dynamic properties. We conclude that this model is applicable to simulate all quantities and polymeric systems as the original BFM does, but with a significant upspeed.

CPP 59: Focus Session: Slow Dynamics in Glasses and Granular Matter II (original: DY, joined by CPP, DF)

The transition into an amorphous solid state is typically accompanied by the observation of slow dynamics. The understanding of such transitions from first principles has seen progress in many of its aspects recently, including nonlinear response, residual stresses, and non-affine deformations. The Focus Session provides an overview of common phenomena and of general concepts in the physical picture of disordered materials. (Organizers M. Sperl and A. Zippelius)

Time: Friday 9:30–12:15

Location: HÜL 186

Invited Talk CPP 59.1 Fri 9:30 HÜL 186
Critical Rheology of Weakly Vibrated Granular Media — ●MARTIN VAN HECKE — Huygens-Kamerlingh Onnes Lab, Leiden University

We experimentally probe the rheology of weakly vibrated granular media, and show that much of it is controlled by a nontrivial 2nd order-like critical point that occurs at finite stress and vibration strength. Close to this critical points, fluctuations become strong, correlation times diverge, and the flow curves exhibit scaling. For smaller vibrations, a 1st order transition emerges which separates a glassy phase from a rapidly flowing phase.

CPP 59.2 Fri 10:00 HÜL 186

THz scattering from granular media — ●PHILIP BORN¹, HEINZ-WILHELM HÜBERS², NICK ROTHBART², and MATTHIAS SPERL¹ — ¹DLR Institute of Materials Physics in Space, Cologne, Germany — ²DLR Institute of Planetary Research, Berlin, Germany

The structure and dynamics of driven dissipative granular media seems to be captured well by simulations. However, the results still evade experimental verification. The dynamics in colloidal suspension in contrast can be investigated comprehensively using light scattering techniques. The particle sizes in common experimental realisations of dense driven granular media, usually with particle sizes above 0.1mm, prevent application of imaging methods and established light scattering methods. Here we present approaches to the structure and dynamics of granular media using THz radiation based light scattering. The matched wavelength ensures high sensitivity to geometric features of granular particle packings and paves the way for in-situ investigations of driven granular media.

CPP 59.3 Fri 10:15 HÜL 186

Correlations and response in sheared hard sphere glasses — ●SUVENDU MANDAL¹, DIERK RAABE¹, and FATHOLLAH VARNIK² — ¹Max-Planck Institut für Eisenforschung, Max-Planck Str. 1, 40237 Düsseldorf, Germany — ²Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr University Bochum, Universitätsstr. 150, 44801 Bochum, Germany

Via event-driven molecular dynamics simulations, we study the packing-fraction and shear-rate dependence of single-particle fluctuations and dynamic correlations in hard-sphere glasses under shear [1]. At packing fractions above the glass transition, correlations increase as shear rate decreases: the exponential tail in the distribution of single-particle jumps broadens and dynamic four-point correlations increase. Interestingly, however, upon decreasing the packing fraction, a broadening of the exponential tail is also observed, while dynamic heterogeneity is shown to decrease. An explanation for this behavior is proposed in terms of a competition between shear and thermal fluctuations. We further address the issue of anisotropy of the dynamic correlations [2,3].

[1] Suvendu Mandal, Markus Gross, Dierk Raabe, and Fathollah Varnik, PRL. 108, 098301 (2012). [2] Suvendu Mandal, Vijaykumar Chikkadi, Bernard Nienhuis, Dierk Raabe, Peter Schall, and Fathollah Varnik, PRE. 88, 022129 (2013). [3] Vijaykumar Chikkadi, Suvendu Mandal, Bernard Nienhuis, Dierk Raabe, Peter Schall, and Fathollah Varnik, EPL. 100, 56001 (2012).

CPP 59.4 Fri 10:30 HÜL 186

Granular matter composed of shape-anisotropic grains under shear — RALF STANNARIUS¹, SANDRA WEGNER¹, TAMÁS BÖRZSÖNYI², and ●BALÁZS SZABÓ² — ¹Inst. of Experimental Physics, University of Magdeburg, Germany, — ²Institute for Solid State Physics and Optics, HAS, Budapest, Hungary

This contribution establishes a link between two different soft matter systems that can develop orientational order, liquid crystals and gran-

ular matter. We present shear experiments with prolate (ellipsoids, cylinders) and oblate (lentils) particles and discuss the observed order and alignment. Positions and orientations of the individual grains in the bulk are resolved by X-ray tomography. Shear experiments show that many observations are qualitatively and even quantitatively comparable to the behavior of the well-understood molecular liquid crystal mesophases, even though the types of interactions are completely different. We establish a quantitative relation between shear alignment and aspect ratio and investigate the interrelations to shear dilatancy and macroscopic friction properties. Long-range effects like particle rearrangements by creeping motion far from the shear band are detected.

15 min. break

Invited Talk CPP 59.5 Fri 11:00 HÜL 186
A Granular Ratchet: Spontaneous Symmetry Breaking and Fluctuation Theorems in a Granular Gas — ●DEVARAJ VAN DER MEER¹, SYLVAIN JOUBAUD², PETER ESHUIS¹, KO VAN DER WEELE³, and DETLEF LOHSE¹ — ¹University of Twente, The Netherlands — ²ENS and University of Lyon, France — ³University of Patras, Greece

We construct a ratchet of the Smoluchowski-Feynman type, consisting of four vanes that are allowed to rotate freely in a vibrofluidized granular gas. The necessary out-of-equilibrium environment is provided by the inelastically colliding grains, and the equally crucial symmetry breaking by applying a soft coating to one side of each vane. The onset of the ratchet effect occurs at a critical shaking strength via a smooth, continuous phase transition. For very strong shaking the vanes interact actively with the gas and a convection roll develops, sustaining the rotation of the vanes. From the experimental results we show that a steady state fluctuation relation holds for the work injected to the system, and that its entropy production satisfies a detailed fluctuation theorem. Surprisingly, we find that the above relations are satisfied to some extent even when a convection roll has developed and there exists a strong coupling between the motion of the vanes and the granular gas.

CPP 59.6 Fri 11:30 HÜL 186

Granular Microrheology in the Large Force Regime — ●TING WANG¹, MATTHIAS GROB², ANNETTE ZIPPELIUS², and MATTHIAS SPERL¹ — ¹Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln — ²Georg-August-Universität Göttingen, Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen

When pulling a particle in a driven granular system with constant force F , the probe particle may approach a steady velocity v . In the large force regime, it was found in our recent simulation that the effective friction coefficient F/v increases with increasing F , being proportional to the square-root of F , while some earlier Brownian dynamics simulations and theories predicted constant friction coefficient. Here, we study the behavior in granular microrheology by a schematic model of mode-coupling theory (MCT) and a simple kinetic theory. Our schematic model qualitatively reproduces the increase of friction tendency but fails to exhibit the square-root law. In the low density limit, the square-root law can be derived from the kinetic theory, based on which, we clarify the discrepancy of the large force behaviors in driven granular systems and Brownian ones.

CPP 59.7 Fri 11:45 HÜL 186

Integration Through Transients Approach to the Rheology of a Sheared Granular Fluid — ●TILL KRANZ¹, FABIAN FRAHSA², MATTHIAS FUCHS², MATTHIAS SPERL³, and ANNETTE ZIPPELIUS¹ — ¹Institut für Theoretische Physik, Universität Göttingen — ²Fachbereich Physik, Universität Konstanz — ³Institut für Mate-

rialphysik im Weltraum, DLR Köln

We generalize the Integration through Transients (ITT) formalism to the non-equilibrium stationary state of randomly driven inelastic hard spheres. ITT was first developed for Brownian suspensions [1] and recently extended to thermostated Newtonian systems [2]. As a result we get generalized Green-Kubo-relations and an equation of motion for the transient density correlator.

Since the seminal work of Bagnold [3] it has been recognized that dissipative hard spheres (i.e. granular particles) have an unusual rheology. In particular, the shear stress σ varies with the square of the shear rate $\dot{\gamma}$, i.e., Bagnold scaling, $\sigma = \eta\dot{\gamma}^2$, holds. We will discuss the response to shear and the dependence on the degree of inelasticity and packing fraction. This includes the transient density correlator and the prefactor, η , of the Bagnold scaling relation. We will comment on the relation to the elastic [1,2] and the unsheared case [4], clarifying how Bagnold scaling emerges.

[1] M. Fuchs, M. E. Cates, *J. Rheol.* **53**, 957 (2009)

[2] K. Suzuki, H. Hayakawa, *Phys. Rev. E* **87**, 012304 (2013)

[3] R. A. Bagnold, *Proc. R. Soc. Lond. A* **225**, 49 (1954)

[4] W. T. Kranz, *et al.*, *Phys. Rev. E* **87**, 022207 (2013)

CPP 59.8 Fri 12:00 HÜL 186

Nonlinear rheology of colloidal systems with attractive interactions: A mode-coupling theory analysis — ●MADHU PRIYA and THOMAS VOIGTMANN — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, Germany

Hard spheres with a short-ranged attraction are a model system for colloid-polymer mixtures. These systems display two separate glasses, attractive and repulsive, connected with glass-glass transitions and higher-order glass-transition singularities. We study the nonlinear rheology of the square-well system in the vicinity of the glass-glass transition, using mode-coupling theory (MCT) in an isotropic-shear approximation. The yield strength and yield strains are studied, depending on packing fraction, attraction range, and strength. The findings of the model are compared with the observations made by recent experiments and computer simulation studies for colloid-polymer systems.

CPP 60: Organic Semiconductors: Material Properties (original: HL, joined by CPP,DS)

Time: Friday 10:15–12:30

Location: POT 051

CPP 60.1 Fri 10:15 POT 051

Pressure dependent Electronic Structure from First Principles — ●FRANZ KNUTH¹, CHRISTIAN CARBOGNO¹, VOLKER BLUM^{1,2}, and MATTHIAS SCHEFFLER¹ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — ²MEMS Department, Duke University, Durham, NC, USA

The electronic properties of organic semiconductors typically exhibit a significant dependence on the strain, stress and pressure [1]. To clarify the role of these effects electronic-structure theory is uniquely suited. However, standard density-functional theory approaches that neglect van-der-Waals interactions and that treat exchange and correlation in a semi-local approximation often fail to describe organic materials properly. To overcome this limitation, we have extended our implementation of the analytical strain derivatives (stress tensor) to include the contributions that stem from (a) the van-der-Waals interaction [2] and (b) the Fock-exchange in hybrid functionals. We discuss the details of our implementation that is based on a local resolution of identity (LVI) of the Coulomb matrix [3]. We validate our approach by investigating the geometric and electronic changes that occur in polyacetylene, polyaniline, and anthracene under pressure. We show that the fraction of exact exchange included in the calculations is critical – and non-trivial to choose – for a correct description of these systems.

[1] J. H. Kim, S. Seo, and H. H. Lee, *Appl. Phys. Lett.* **90**, 143521 (2007).

[2] A. Tkatchenko, and M. Scheffler, *PRL* **102**, 073005 (2009)

[3] A. Sodt, and M. Head-Gordon, *J. Chem. Phys.* **128**, 104106 (2008)

CPP 60.2 Fri 10:30 POT 051

DFT study of vibronic properties of partially fluorinated nickel phthalocyanine — ●DAVOUD POULADSAZ — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Since fluorinated phthalocyanines are shown to be sensitive to reducing gases due to the withdrawing effect of fluorine atoms, by means of density functional theory, we have investigated the effect of fluorination on the vibronic couplings and ionization potential in nickel phthalocyanine.

CPP 60.3 Fri 10:45 POT 051

Ab-initio investigation of Charge and Spin transport properties of Organic Semiconductors. — ●SANDIP BHATTACHARYA and STEFANO SANVITO — School of Physics and CRANN, Trinity College Dublin, Ireland

In this talk I will describe in detail our procedure to explore the spin and charge transport properties of organic single-crystal semiconductors from first principles. Our technique involves representing the organic semiconductor with a tight-binding model, including coupling of the charge carrier to phonons and spin relaxation due to hyperfine and spin-orbit coupling interaction. The ab-initio Hamiltonian parameters are extracted from DFT and the maximally localized Wannier functions scheme. We evolve the classical fields in the Hamiltonian via Monte Carlo simulations, and then compute the mobility from Kubo

formula and the spin-diffusion length from a Landauer-Büttiker approach. We shall demonstrate calculated charge carrier mobilities very close to those measured in single-crystal rubrene-based organic field effect transistors and spin-diffusion length quite close to that estimated in experiments on rubrene-based spin valves. In the second part of my talk, I shall discuss the use of a similar procedure to predict the ab-initio spin and charge transport characteristics of Triarylamine-based organic nanowires, recently synthesized. We obtain quite superior estimates for hole mobilities as well as spin-diffusion lengths in such organic nanowires, corroborating the experimental find of exceptional conductance through nanodevices made out of such nanowires.

CPP 60.4 Fri 11:00 POT 051

Growth control of AgTCNQ nanowire arrays by using template-assisted electro-deposition method — ●CHENGLIANG WANG¹, LIAOYONG WEN¹, THOMAS KUPS², RANJITH VELLACHERI¹, YAOGUO FANG¹, PETER SCHAAF², HUAPING ZHAO¹, and YONG LEI¹ — ¹Institute for Physics and IMN MacroNano(ZIK), Ilmenau University of Technology, Ilmenau 98693, Germany — ²Institute of Materials Engineering and IMN MacroNano(ZIK), Ilmenau University of Technology, Ilmenau 98693, Germany

One dimensional (1D) organic semiconductor nanostructures, especially their aligned arrays, have attracted extensive attention due to their potential application in organic optoelectronics, and template-assisted methods have been proved to be one of the most powerful methods to achieve this kind of arrays. Due to the small size of the AAO nanopores, diffusion of the objects into the nanopores is one of the crucial issues to achieve nanowire arrays. Here, the growth control of AgTCNQ (TCNQ: 7,7,8,8-tetracyanoquinodimethane) nanowire arrays is achieved by using template-assisted electro-deposition methods. We find that the diffusion of the electrolyte into the nanopores takes an important role in the electro-deposition process and the equilibrium between the reduction and the diffusion is necessary to achieve continuous AgTCNQ nanowire arrays. We believed that the analysis of the equilibrium between the deposition and the diffusion and the controllable synthesis of organic semiconductor arrays will benefit the preparation of other semiconductor arrays.

CPP 60.5 Fri 11:15 POT 051

Energy-transfer in ZnO/ladder-type oligophenylenes hybrid structures — ●FRANCESCO BIANCHI¹, SYLKE BLUMSTENGEL¹, FRITZ HENNEBERGER¹, BJÖRN KOBIN², STEFAN HECHT², RAFFAEL SCHLESINGER¹, and NORBERT KOCH¹ — ¹Institut für Physik Humboldt-Universität, Berlin, Germany — ²Department of Chemistry Humboldt-Universität, Berlin, Germany

Inorganic/organic hybrid systems designed to inherit the advantageous properties of each of their constituents are of great interest both to basic science as well as for optoelectronic applications. In this regard it is required to find an organic material that exhibits specific properties like narrow transitions, large dipole moment, small emission-absorption Stokes shift and an optical gap that corresponds

to the inorganic material. The design we use consists in a three spiro-bridged ladder-type quarter-phenyl (SP3-L4P) grown on ZnO-based single quantum wells (SQW) to obtain incoherent coupling. In such a setting, it should be possible to convert Wannier excitons of the SQW into Frenkel excitons of the organic layer via a Förster type energy transfer (FRET).

We investigate the FRET between SQW with different cap thickness and a 3Sp-L4P thin layer evaporated on top of them. With photoluminescence excitation and time-resolved spectroscopy we demonstrate that these hybrid structures exhibit energy transfer with an efficiency up to 65%. Despite the high efficiency, UPS measurements show a type II interface between ZnO and the molecules layer, leading to a charge separation process that limits the light emitted. Finally we investigate on the use of high gap material spacer to reduce this effect.

CPP 60.6 Fri 11:30 POT 051

Temperature dependent PL measurements of rubrene single crystals with μm -resolution — ●T. SCHMEILER¹, J. GABEL¹, R. CLAESSEN¹, and J. PFLAUM^{1,2} — ¹Inst. Exp. Phys. VI/IV, University of Würzburg, 97074 Würzburg — ²ZAE Bayern e.V., 97074 Würzburg

Our previous demonstration of spatial confinement effects on exciton dynamics in rubrene (rub) single crystals, microcrystals and amorphous films [1] has raised fundamental questions on excitonic processes occurring at surfaces and interfaces of molecular stacks. We address this topic by analyzing the temperature dependent PL characteristics of rub single crystals on μm -length scales and under various boundary condition by e.g. capping them with thin films of different polarizability such as Au or LaVO. At first, a pronounced enhancement of the total PL intensity of up to two orders of magnitudes was observed in case of the Au top layer which can be attributed to a resonant coupling of the excited rub states to the surface plasmon modes of the metal. This coupling phenomenon is further corroborated by relative intensity changes within the PL spectra of the Au covered rub upon cooling below 100K. In case of a LaVO capping layer, providing high polarizability without significant contributions by exciton quenching, a strong temperature dependent influence in the rub PL peaks at short wavelengths is observed. This behavior will be discussed in the context of temperature dependent changes of the LaVO layer itself as well as different coupling mechanism for the interfacial excitonic species. Financial support by the DFG research unit FOR 1809 (project PF385/6) is gratefully acknowledged. [1] B. Giesekeing et al., arXiv:1309.1107

CPP 60.7 Fri 11:45 POT 051

Optical absorption and photoluminescence properties of perylene single-crystals — ●ANDRE RINN, NIKLAS KRAUS, ANDRÉ PICK, GREGOR WITTE, and SANGAM CHATTERJEE — Phillips Universität Marburg, Marburg, Germany

Organic semiconductors are considered promising candidates for next-generation optical devices. However, a detailed systematic understanding of the electro-optical response is in a much less holistic state than for inorganic materials such as Si or GaAs. Therefore, we investigated the two crystalline phases of perylene as model organic semiconductors and gain further insight in their optical response. This system crystallizes in two different phases: the beta-phase has a monomeric herringbone structure with two molecules per primitive unit cell, whereas the alpha phase grows in a dimeric herringbone configuration with four molecules per unit cell. The single-crystalline samples have been grown in silicon oil, which results in microcrystals of excellent quality. Hence, we can investigate the consequences of the respective crystal orientation on the Davydov splitting of the excitons as well as excimer formation. Both configurations have been investigated with polariza-

tion resolved absorption spectroscopy and time resolved luminescence experiments. Absorption spectroscopy reveals results with significant deviations from the widespread Davydov picture. The data obtained by time resolved luminescence shows characteristic excimer behavior. Additionally, the optical spectra are compared to the response of perylene in solution and the vapour phase.

CPP 60.8 Fri 12:00 POT 051

Direct measurement of the charge carrier mobility in organic donor-acceptor blend in device geometry – including extreme stoichiometry — ●JOHANNES WIDMER¹, JANINE FISCHER¹, CHRISTIAN KOERNER¹, KARL LEO¹, and MORITZ RIEDE^{1,2} — ¹Institut für Angewandte Photophysik (IAPP), TU Dresden, Germany — ²Current address: Clarendon Laboratory, UK

Blend layers of an organic donor (D) and a fullerene acceptor (A) are a key component of highly efficient organic solar cells. The charge carrier mobility in the blend sensibly affects the device efficiency concerning transport and recombination of charge carriers.

The applied method “POEM” – potential mapping by thickness variation – is a direct measurement giving model-free experimental access to the effective mobility $\mu(F, n)$ as a function of the electric field F and the charge carrier density n . It is based on a novel evaluation strategy for space-charge limited current (SCLC) in single carrier devices in a vertical device geometry.[Widmer et al., Org. El. (2013)]

Here, we apply POEM to characterize the hole transport in D:A blends of small molecules with different blend ratios. The measurements cover common ratios as well as strongly diluted blends with only $\approx 1\%$ donor content, which are known to yield efficient solar cells. Beyond characterizing disorder and trap states, which influence μ , the POEM measurements reveal that also in the diluted blend effective hole transport is possible, but takes place not only on the donor.

The obtained $\mu(F, n)$ functions allow for an advanced understanding of charge transport in D:A blends – also in moderate blend ratios.

CPP 60.9 Fri 12:15 POT 051

Polymer aggregation control in polymer: PCBM bulk heterojunctions adapted from solution — ●CHRISTIAN KÄSTNER¹, DANIEL EGBE², and HARALD HOPPE¹ — ¹Ilmenau University of Technology, Ilmenau, Germany — ²Linz Institute for Organic Solar Cells, Linz, Austria

It is common knowledge that the polymer conformation and its phase separation with fullerene derivatives are delicate issues crucially impacting on the photovoltaic parameters of polymer based solar cells. Whereas strongly intermixed polymer:fullerene phases provide large interfacial area and consequently a high quantum efficiency of exciton dissociation, pristine and primarily ordered polymer and fullerene domains support efficient charge transport and percolation. To study the aggregation and phase separation in polymer solar cells we investigated counterbalancing influences of polymer solution concentration and PCBM ([6,6]-phenyl-C61-butyric acid methyl ester) blending ratio on the basis of a semi-crystalline anthracene-containing poly(p-phenylene-ethynylene)-alt-poly(p-phenylene-vinylene) (PPE-PPV) copolymer statistically bearing either branched 2-ethylhexyloxy or linear octyloxy side-chains (AnE-PVstat). The polymer aggregation varied with both, solution and PCBM concentrations, yielding a specific maximum within the parameter range. We explicitly demonstrate the counterbalancing effect on charge generation and transport for increasing polymer aggregation. Furthermore the influence of polymer aggregation on fundamental optoelectronic properties is discussed, providing detailed understanding of resulting photovoltaic parameters.