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

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## Overview of Invited Talks and Sessions

(Lecture rooms: C 130, C 243, C 264, and PC 203; Posters: A, B, and C)

### Invited Talks

| | | | | |
|---|---|---|---|---|
| CPP 2.1 | Mon | 9:30–10:00 | C 264 | **Polymer films with optically controlled shape and functionality on a nanometer scale** — •Svetlana Santer |
| CPP 2.6 | Mon | 11:15–11:45 | C 264 | **Field Responses of Magnetic Gels** — Rudolf Weeber, Sofia S. Kantorovich, •Christian Holm |
| CPP 3.6 | Mon | 10:45–11:15 | C 243 | **Functional Nanocomposites: Disordered media with a cooperative macroscopic action** — •Mady Elbahri |
| CPP 6.3 | Mon | 10:00–10:30 | PC 203 | **Direct observation of prefreezing at the interface melt-solid in polymer crystallization** — Ann-Kristin Löhmann, Thomas Henze, •Thomas Thurn-Albrecht |
| CPP 13.5 | Mon | 16:00–16:30 | C 264 | **Magnetic particles in polymer harness: Modeling mesoscopic magnetomechanics of polymer composites** — •Yuriy Raikher, Oleg Stolbov |
| CPP 14.4 | Mon | 16:30–17:00 | PC 203 | **Spontaneous symmetry breaking in 2D: Kibble-Zurek mechanism in colloidal monolayers at finite cooling rates** — Sven Deutschländer, Georg Maret, •Peter Keim |
| CPP 26.1 | Tue | 14:00–14:30 | C 130 | **Ultrafast Coherent Charge Transfer in Solar Cells and Artificial Light Harvesting Systems** — •Christoph Lienau, Ephraim Sommer, Antonietta de Sio, Ralf Vogelgesang, Margherita Maiuri, Giulio Cerullo, Angel Rubio, Carlo A. Rozzi, Elisa Molinari |
| CPP 27.1 | Tue | 14:00–14:30 | C 243 | **Structure formation at interfaces: breath figures and beyond** — •Masoud Amirkhani |
| CPP 38.1 | Wed | 9:30–10:00 | C 264 | **Challenges for the development of coarse-grained simulation models for complex soft matter systems** — •Christine Peter |
| CPP 38.8 | Wed | 11:45–12:15 | C 264 | **Answering old questions with new simulation methods: what is the behavior of fluctuation spectra and Frank constants in polymer nematics?** — •Kostas Daoulas, Patrick Gemünden |
| CPP 52.1 | Wed | 15:00–15:30 | C 130 | **Ultraslow dynamics of hydrated metal ions at the water-solid interface observed by atomic force microscopy** — •Kislon Voitchovsky |
| CPP 52.6 | Wed | 16:45–17:15 | C 130 | **Water flow along a solid interface affects the Stern layer** — •Mischa Bonn |
| CPP 55.1 | Wed | 15:00–15:30 | C 264 | **A new perspective of materials processing** — •Kyung Hyun Ahn |
| CPP 58.1 | Wed | 15:45–16:15 | PC 203 | **The Tricontinuous 3ths(5) Phase: A New Morphology in Copolymer Melts** — •Gerd Schroeder-Turk, Michael Fischer, Liliana de Campo, Jacob Kirkensgaard, Stephen Hyde |
| CPP 60.1 | Thu | 9:30–10:00 | C 130 | **Advances in hybrid solar cells: From hybrid organic/inorganic to perovskite photovoltaics** — •Lukas Schmidt-Mende |
| CPP 60.7 | Thu | 11:30–12:00 | C 130 | **The solid state physics of hybrid perovskites** — •Jarvist Moore Frost, Federico Brivio, Keith Butler, Aurelien Leguy, Artem Bakulin, Piers Barnes, Aron Walsh |
| CPP 61.1 | Thu | 9:30–10:00 | C 243 | **Flow instabilities in soft glassy materials** — •Suzanne Fielding |
| CPP 61.5 | Thu | 10:45–11:15 | C 243 | **Dense granular flow** — •Annette Zippelius |

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| CPP 68.1 | Thu | 15:00–15:30 | C 130 | **Photophysics of organic-inorganic hybrid lead iodide perovskite single crystals** — •Maria Antonietta Loi |
| CPP 68.2 | Thu | 15:30–16:00 | C 130 | **Exciton stabilization in hybrid lead-halide perovskites: photophysical versus structural properties** — •Annamaria Petrozza |
| CPP 72.1 | Thu | 15:45–16:15 | PC 203 | **Flagellar synchronisation through direct hydrodynamic interactions** — •Marco Polin, Douglas Brumley, Kirsty Wan, Raymond Goldstein |
| CPP 72.2 | Thu | 16:15–16:45 | PC 203 | **Active motion: From single microswimmers to their emergent collective behavior** — •Holger Stark |
| CPP 73.1 | Thu | 15:30–16:00 | C 243 | **Microscopic flows of complex suspensions** — •Anke Lindner |
| CPP 74.1 | Thu | 17:00–17:30 | C 243 | **Multiscale Contact Mechanics for Rough Surfaces with Applications to Rubber Friction and the Leak-rate of Rubber Seals** — •Bo Persson |
| CPP 76.1 | Fri | 9:30–10:00 | C 130 | **Strong and switchable magnetic couplings in molecular semiconductor films** — •Michele Serri, Wei Wu, Luke Fleet, Cyrus Hirjibehedin, Nicholas Harrison, Chris Kay, Andrew Fisher, Gabriel Aeppli, Sandrine Heutz |
| CPP 76.7 | Fri | 11:30–12:00 | C 130 | **Excitonic phenomena in molecular semiconductors** — •Jens Pflaum |
| CPP 79.1 | Fri | 9:30–10:00 | C 264 | **From chemical nanomotors to biological microswimmers** — •Peer Fischer |

## Invited talks of the joint symposium SYOP

See SYOP for the full program of the symposium.

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| SYOP 1.1 | Mon | 15:00–15:30 | H 0105 | **Formation mechanisms of covalent nanostructures** — •Jonas Björk |
| SYOP 1.2 | Mon | 15:30–16:00 | H 0105 | **Selective C-H Activation and C-C coupling on Metal Surfaces** — •Lifeng Chi |
| SYOP 1.3 | Mon | 16:00–16:30 | H 0105 | **On-Surface Synthesis on Insulating Substrates** — •Angelika Kuehnle |
| SYOP 1.4 | Mon | 16:45–17:15 | H 0105 | **On-surface polymerization - a synthetic route to 2D polymers** — •Markus Lackinger |
| SYOP 1.5 | Mon | 17:15–17:45 | H 0105 | **On-surface azide-alkyne click chemistry and a novel metal-organic network based on Cu adatom trimers** — •Trolle Linderoth |

## Invited talks of the joint symposium SYME

See SYME for the full program of the symposium.

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| SYME 1.1 | Fri | 9:30–10:00 | H 0105 | **Excitations and charge transfer phenomena in C based systems** — •Elisa Molinari |
| SYME 1.2 | Fri | 10:00–10:30 | H 0105 | **Towards optimal correlation factors for many-electron perturbation theories** — •Andreas Grüneis |
| SYME 1.3 | Fri | 10:30–11:00 | H 0105 | **Towards an ab-initio description of high temperature superconductivity** — •Garnet Chan |
| SYME 1.4 | Fri | 11:15–11:45 | H 0105 | **Correlation effects in unconventional superconductors: from micro- to nano- and macroscales.** — •Roser Valenti |
| SYME 1.5 | Fri | 11:45–12:15 | H 0105 | **Stochastic density functional and GW theories scaling linearly with system size** — •Roi Baer, Daniel Neuhauser, Eran Rabani |

## Sessions

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| CPP 1.1–1.12 | Mon | 9:30–12:45 | C 130 | **Colloids and Complex Liquids I (joint session CPP, BP, DY)** |
| CPP 2.1–2.9 | Mon | 9:30–12:30 | C 264 | **Focus: Field Controllable Functional Polymers I** |
| CPP 3.1–3.12 | Mon | 9:30–13:00 | C 243 | **Nanoparticles and Composite Materials I (joint session CPP, BP)** |
| CPP 4.1–4.9 | Mon | 9:30–12:15 | BH-N 243 | **Statistical Physics in Biological Systems (joint session DY, BP, CPP)** |
| CPP 5.1–5.9 | Mon | 9:30–12:00 | BH-N 334 | **Anomalous Diffusion (joint session DY, CPP)** |
| CPP 6.1–6.7 | Mon | 9:30–11:30 | PC 203 | **Crystallization, Nucleation and Self Assembly I (joint session CPP, DY)** |

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| CPP 7.1–7.14 | Mon | 9:30–13:00 | H 2032 | **Organic Electronics and Photovoltaics** |
| CPP 8.1–8.14 | Mon | 15:00–18:45 | C 130 | **Colloids and Complex Liquids II (joint session CPP, BP, DY)** |
| CPP 9.1–9.14 | Mon | 15:00–18:45 | C 243 | **Nanoparticles and Composite Materials II (joint session CPP, BP)** |
| CPP 10.1–10.5 | Mon | 15:00–17:45 | H 0105 | **On-surface Polymerization** |
| CPP 11.1–11.13 | Mon | 15:00–18:45 | BH-N 243 | **Brownian Motion and Transport (joint session DY, CPP)** |
| CPP 12.1–12.15 | Mon | 15:00–19:30 | H 2032 | **Organic Thin Films** |
| CPP 13.1–13.12 | Mon | 15:00–18:30 | C 264 | **Focus: Field Controllable Functional Polymers II** |
| CPP 14.1–14.9 | Mon | 15:45–18:30 | PC 203 | **Crystallization, Nucleation and Self Assembly II (joint session CPP, DY)** |
| CPP 15.1–15.15 | Mon | 16:00–19:00 | Poster A | **P1: Interfaces and Thin Films** |
| CPP 16.1–16.13 | Tue | 9:30–13:00 | C 130 | **Organic Electronics and Photovoltaics: Transport of Charges - from Molecules to Devices (joint session with HL, TT)** |
| CPP 17.1–17.11 | Tue | 9:30–12:30 | BH-N 128 | **Microswimmers (joint session DY, BP, CPP)** |
| CPP 18.1–18.2 | Tue | 9:30–10:00 | C 243 | **On-Surface Polymerization (contributed session to SYOP, joint session CPP, MI)** |
| CPP 19.1–19.10 | Tue | 9:30–12:15 | A 053 | **Transport: Graphene (joint session TT, CPP, DS, DY, HL, MA, O)** |
| CPP 20.1–20.10 | Tue | 9:30–12:30 | H 1028 | **Membranes and vesicles I (joint session BP, CPP)** |
| CPP 21.1–21.13 | Tue | 9:30–13:00 | C 264 | **Polymer dynamics** |
| CPP 22.1–22.8 | Tue | 9:30–11:30 | PC 203 | **Charged Soft Matter I** |
| CPP 23.1–23.9 | Tue | 10:00–12:30 | C 243 | **Interfaces and Thin Films I (joint session CPP, DS)** |
| CPP 24.1–24.5 | Tue | 10:30–12:30 | HE 101 | **Focus session: Structure, chemistry, and ion solvation at solid-liquid interfaces I (joint session O, CPP)** |
| CPP 25.1–25.4 | Tue | 14:00–16:00 | HE 101 | **Focus session: Structure, chemistry, and ion solvation at solid-liquid interfaces II (joint session O, CPP)** |
| CPP 26.1–26.7 | Tue | 14:00–16:00 | C 130 | **Organic Electronics and Photovoltaics: OPV I (joint session CPP, HL, TT)** |
| CPP 27.1–27.7 | Tue | 14:00–16:00 | C 243 | **Interfaces and Thin Films II (joint session CPP, DS)** |
| CPP 28.1–28.8 | Tue | 14:00–16:00 | C 264 | **New Instruments and Methods** |
| CPP 29.1–29.7 | Tue | 14:30–16:15 | BH-N 243 | **Reaction-Diffusion Systems (Joint session DY, CPP)** |
| CPP 30.1–30.19 | Tue | 14:00–16:00 | Poster B | **P2: Organic Electronics and Photovoltaics** |
| CPP 31.1–31.8 | Tue | 14:00–16:00 | Poster B | **P3: Hybrid Photovoltaics and Preovskites** |
| CPP 32.1–32.15 | Tue | 14:00–16:00 | Poster B | **P4: Computational Physics of Soft Matter** |
| CPP 33.1–33.8 | Tue | 14:00–16:00 | Poster C | **P5: Microswimmers, Active Liquids** |
| CPP 34.1–34.10 | Tue | 14:00–16:00 | Poster C | **P6: Biomaterials and Biopolymers** |
| CPP 35.1–35.5 | Tue | 14:00–16:00 | Poster C | **P7: Hydrogels and Elastomers** |
| CPP 36.1–36.13 | Wed | 9:30–13:00 | C 130 | **Organic Electronics and Photovoltaics: OPV II (joint session CPP, HL, TT)** |
| CPP 37.1–37.13 | Wed | 9:30–13:00 | C 243 | **Interfaces and Thin Films III (joint session CPP, DS)** |
| CPP 38.1–38.11 | Wed | 9:30–13:00 | C 264 | **Computational Physics of Soft Matter I** |
| CPP 39.1–39.12 | Wed | 9:30–13:15 | H 1058 | **Cell adhesion, mechanics and migration I (Joint session BP, CPP)** |
| CPP 40.1–40.8 | Wed | 9:30–11:30 | PC 203 | **Charged Soft Matter II** |
| CPP 41.1–41.4 | Wed | 9:30–11:00 | EB 407 | **Optical and Nonlinear Optical Properties I (joint session DF, CPP)** |
| CPP 42.1–42.5 | Wed | 11:30–12:45 | H 3005 | **Transport: Fluctuations and Noise (joint session TT, CPP, DY)** |
| CPP 43.1–43.26 | Wed | 10:00–13:00 | Poster A | **P8: Nanoparticles and Compsite Materials** |
| CPP 44.1–44.13 | Wed | 10:00–13:00 | Poster A | **P9: Crystallization, Nucleation and Self Assembly** |
| CPP 45.1–45.13 | Wed | 10:00–13:00 | Poster A | **P10: Colloids and Complex Liquids** |
| CPP 46.1–46.20 | Wed | 10:00–13:00 | Poster A | **P11: Wetting, Micro and Nano Fluidics** |
| CPP 47.1–47.4 | Wed | 10:00–13:00 | Poster A | **P12: Glasses and Glass Transition** |
| CPP 48.1–48.8 | Wed | 10:00–13:00 | Poster A | **P13: Charged Soft Matter** |
| CPP 49.1–49.6 | Wed | 10:00–13:00 | Poster A | **P14: Polymer Dynamics** |
| CPP 50.1–50.7 | Wed | 10:00–13:00 | Poster A | **P15: Polymers and Fields** |
| CPP 51.1–51.5 | Wed | 10:00–13:00 | Poster A | **P16: New Instruments and Methods** |
| CPP 52.1–52.9 | Wed | 15:00–18:00 | C 130 | **Focus: Electrolytes at Interfaces - Stern Layer (joint session with CPP, BP)** |

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| CPP 53.1–53.12 | Wed | 15:00–18:15 | HE 101 | **Inorganic/organic interfaces: Electronic properties II (joint session O, CPP)** |
| CPP 54.1–54.12 | Wed | 15:00–18:15 | C 243 | **Wetting, Micro and Nanofluidics (joint session CPP, DY)** |
| CPP 55.1–55.12 | Wed | 15:00–18:30 | C 264 | **Flow-Induced Structures in Complex Fluids (with DRG, Deutsche Rheologische Gesellschaft, and DY)** |
| CPP 56.1–56.12 | Wed | 15:00–18:30 | H 1028 | **Membranes and vesicles II (joint session BP, CPP)** |
| CPP 57.1–57.7 | Wed | 15:00–16:45 | BH-N 333 | **Complex Fluids and Soft Matter - Part I (joint session DY, CPP, BP)** |
| CPP 58.1–58.10 | Wed | 15:45–18:30 | PC 203 | **Computational Physics of Soft Matter II** |
| CPP 59 | Wed | 18:30–19:30 | C 130 | **CPP Mitgliederversammlung** |
| CPP 60.1–60.11 | Thu | 9:30–13:00 | C 130 | **Focus Session Hybrid Photovoltaics and Prevovskites I (joint session CPP HL, O)** |
| CPP 61.1–61.11 | Thu | 9:30–13:00 | C 243 | **Focus: Disordered Systems, Glasses under Shear I (joint session CPP, DY)** |
| CPP 62.1–62.7 | Thu | 9:30–11:45 | BH-N 334 | **Complex Fluids and Soft Matter - Part II (joint session DY, CPP, BP)** |
| CPP 63.1–63.11 | Thu | 9:30–13:00 | H 1028 | **Cytoskeletal filaments (Joint session BP, CPP)** |
| CPP 64.1–64.9 | Thu | 9:30–12:00 | C 264 | **Flow-Induced Structures in Complex Fluids (with DRG, Deutsche Rheologische Gesellschaft, and DY)** |
| CPP 65.1–65.4 | Thu | 9:30–10:30 | PC 203 | **(Hydro)gels and Elastomers** |
| CPP 66.1–66.6 | Thu | 9:30–11:00 | H 3010 | **Low-Dimensional Systems: Molecular Conductors (joint session with CPP, HL, MA, O)** |
| CPP 67 | Thu | 12:00–13:00 | C 264 | **Mitgliederversammlung der Deutschen Rheologischen Gesellschaft (DRG)** |
| CPP 68.1–68.10 | Thu | 15:00–18:15 | C 130 | **Focus Session Hybrid Photovoltaics and Perovskites (joint session CPP, HL)** |
| CPP 69.1–69.11 | Thu | 15:00–18:00 | C 264 | **Biomaterials and Biopolymers (joint session CPP, BP)** |
| CPP 70.1–70.6 | Thu | 15:00–16:45 | BH-N 334 | **Complex Fluids and Soft Matter - Part III (joint session DY, CPP, BP)** |
| CPP 71.1–71.9 | Thu | 15:00–17:30 | BH-N 128 | **Glasses and Glass transition (joint session DY, CPP, DF)** |
| CPP 72.1–72.7 | Thu | 15:45–18:00 | PC 203 | **Microswimmers, Active Liquids I (joint session CPP, BP, DY)** |
| CPP 73.1–73.5 | Thu | 15:30–17:00 | C 243 | **Focus: Disordered Systems/Glasses under Shear (joint session CPP, DY)** |
| CPP 74.1–74.2 | Thu | 17:00–17:45 | C 243 | **Friction and Lubrication** |
| CPP 75.1–75.2 | Thu | 18:00–18:30 | C 264 | **Physics of Food (joint session CPP, BP)** |
| CPP 76.1–76.7 | Fri | 9:30–12:00 | C 130 | **Organic Electronics and Photovoltaics: Devices (joint session CPP, HL, TT)** |
| CPP 77.1–77.4 | Fri | 9:30–11:30 | BH-N 243 | **Special Session in Honor of the 75th Birthday of Siegfried Hess: Non-equilibrium dynamics of anisotropic fluids (Joint session DY, CPP)** |
| CPP 78.1–78.7 | Fri | 9:30–11:15 | C 243 | **Glasses and Glass Transition (joint session CPP, DF, DY)** |
| CPP 79.1–79.7 | Fri | 9:30–11:30 | C 264 | **Microswimmers, Active Liquids II (joint session CPP, BP, DY)** |
| CPP 80.1–80.10 | Fri | 9:30–12:15 | H 0110 | **Transport: Molecular Electronics (joint session with TT, CPP, HL, MA, O)** |

## Annual General Meeting of the Chemical and Polymer Physics Division

Mittwoch 18:30–19:30 C 130

- Bericht
- Posterpreis (gestiftet von Asylum Research)
- Verschiedenes

# CPP 1: Colloids and Complex Liquids I (joint session CPP, BP, DY)

Time: Monday 9:30–12:45 Location: C 130

CPP 1.1 Mon 9:30 C 130

**Disclination lines at homogeneous and heterogeneous colloids immersed in a chiral liquid crystal** — •Sergej Schlotthauer[1], Michael Melle[1], Carol K. Hall[2], Enrique Diaz-Herrera[3], and Martin Scheon[1,2] — [1]Technische Universität Berlin, Berlin, Germany — [2]North Carolina State University, Raleigh (NC), USA — [3]Universidad Autonoma Metropolitana-Iztapalapa, Iztapalapa , Mexico

We perform Monte Carlo simulations in the isothermal-isobaric ensemble to study defect topologies formed in a cholesteric liquid crystal due to the presence of a spherical colloidal particle. Topological defects arise because of the competition between anchoring at the colloidal surface and the local director. We consider homogeneous colloids with either local homeotropic or planar anchoring to validate our model by comparison with earlier lattice Boltzmann studies. The presence of a Janus colloid in a choleteric host fluid reveals a rich variety of defect structures. Using the Frank free energy we analyze these defects quantitatively indicating a preferred orientation of the Janus colloid relative to the cholesteric helix.

CPP 1.2 Mon 9:45 C 130

**Anisometry versus anisotropy in systems of colloidal magnetic cubes** — •Joe Donaldson[1] and Sofia Kantorovich[1,2] — [1]Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria — [2]Ural Federal University, Lenin av. 51, 620083, Ekaterinburg, Russia

Contemporary colloid science provides numerous ways of synthesising particles with non-spherical geometries. Indeed, a whole spectrum of shapes is now readily accessible, cubes being one such example. The directionally dependent interactions of these particles are key tools in the development of new soft materials. An additional internal anisotropy is introduced into the system when these particles are constructed from a magnetic medium. Consequently, the interplay between anisometry and anisotropy, and its influence on how magnetic particles self-assemble, can be studied. Two different magnetic orientations within the cube have been considered; the first is represented by a dipole aligned along the [001] crystallographic axis, and the second by a dipole aligned along the [111] axis. We have determined the ground state structure of isolated clusters for both systems and have shown for the [001] orientation a preference for a ground state dominated by chain formation. In contrast, clusters of [111] orientated particles tend to arrange in lattices within which dipoles form ring structures consisting of four dipoles. We shall discuss the consequences of these structural configurations on the bulk properties of such systems, including preliminary predictions of the magnetic properties of dilute suspensions.

CPP 1.3 Mon 10:00 C 130

**Active microrheology of a nematic Liquid crystal** — •Tillmann Stieger[1], Andrés Córdoba[2], Marco G. Mazza[3], Juan J. de Pablo[2], and Martin Schoen[1] — [1]Technische Universität Berlin — [2]University of Chicago — [3]MPIDS Göttingen

The knowledge of rheological properties of soft matter is of great importance for a variety of applications such as lubricants or the reduction of friction. The rheology of materials becomes particularly relevant if systems are miniaturized to the nanometer length scale at which physical properties of soft matter are altered significantly from their microscopic bulk properties. The focus of this work are nematic liquid crystals (LC) which are characterized by a high degree of orientational order along a specific direction. If now a colloid is immersed into such a nematic host phase properties of the later are effected greatly at the nanoscale. The colloid perturbs orientational order of the nematic LC in its vicinity. This causes defect topologies to arise. We present nonequilibrium molecular dynamics (MD) simulations of a homogenous colloid with either planar or perpendicular anchoring of LC molecules at the colloid's surface. This leads to well known defect topologies such as the Boojum defect or the Saturn ring. The colloid is moved periodically, comparable to a typical experimental setup where one uses optical tweezers. The phase shift and the magnitude of the measured force response is used to investigate viscoelastic properties of the LC host phase. Specifically, we are interested in calculating the dynamic modulus $G = G' + iG''$, where $G'$ and $G''$ are storage and loss moduli. For both quantities we present analytic expressions that can be used to analyse our MD data.

CPP 1.4 Mon 10:15 C 130

**Characterizing Dissipation during the Crystallization Process** — •Sven Dorosz — 162a avenue de la faiencerie, L1511 Luxemburg

I present computational results on the compression of a hard sphere liquid into the solid phase in finite time.

I will discuss the properties of the resulting work distributions and in particular focus on the correlations between the dissipated heat during the process and the detected structures in the solid resp. melt.

CPP 1.5 Mon 10:30 C 130

**Colloidal Plastic Crystals of Hard Dumbbells under Shear** — •Nils Heptner[1,2], Fangfang Chu[1,2], Matthias Ballauff[1,2], and Joachim Dzubiella[1,2] — [1]Helmholtz-Zentrum Berlin, Germany — [2]Humboldt-Universität zu Berlin, Germany

We study the structural response of plastic crystals of colloidal dumbbells to an oscillatory shear field using Brownian Dynamics (BD) computer simulations. Under increasing shear strains, a discontinuous transition is found from a twinned-fcc like crystal to a partially oriented highly ordered sliding-layer state via a disordered intermediate state. In this novel partially oriented sliding-layer phase, sheared hard dumbbells exhibit a small but finite collective orientational order. We show that the orientations of only weakly anisotropic particles play a crucial role in non-equilibrium transitions. Our findings from simulations are compared to data obtained by rheo-SANS experiments and reveal the nature of a second rheological yielding event which has not been observed for crystalline suspensions of hard spheres.

CPP 1.6 Mon 10:45 C 130

**Experimental determination of structural and dynamical heterogeneities in a metastable colloidal fluid** — Sebastian Golde[1], Markus Franke[2], Thomas Palberg[3], and •Hans Joachim Schöpe[4] — [1]Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany — [2]DB Systel GmbH, Weilburger Straße 22 B4.14, 60326 Frankfurt a. Main — [3]Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, 55128 Mainz, Germany — [4]Eberhards Karls Universität Tübingen, Auf der Morgenstelle 10, 72026 Tübingen, Germany

Metastable fluids exhibit heterogeneous dynamics as well as heterogeneous structure [1]. These dynamical and structural heterogeneities play an important role in the understanding of the glass transition and crystallization. Simulations suggest that these heterogeneities in dynamics and structure are linked, but the direct experimental proof is still lacking [2]. Using space- and time-resolved dynamic light scattering and time-resolved multi angle static light scattering [3], we study the dynamics and structure in a model system of colloidal hard spheres during crystallization and vitrification. For the first time, direct correlation between the temporal evolution of the dynamical heterogeneities and the structural heterogeneities was obtained from an analysis of the subensemble resolved particle dynamics and the evolution of the static structure factor.

[1] L. Berthier and G. Biroli, Rev.s of Mod. Phys., 83, (2011,[2] T. Kawasaki and H. Tanaka, JPCM, 22 (2010),[3] M. Franke, S. Golde and H.J. Schöpe, Soft Matter 10, 5380 (2014)

### 15 min. break

CPP 1.7 Mon 11:15 C 130

**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. Bidisperse 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 density is further increased [2].

To develop a theoretical understanding of all these effects, we simulate hard spheres under pressure-driven flow in two and three dimensions using the mesoscale simulation technique of multi-particle collision dynamics which is an efficient solver of the Navier-Stokes equation and includes thermal motion.

In our simulations, we reproduce the experimental observations that a monodisperse suspension enriches the channel center and a binary mixture segregates into its two species. Comparison with our analytical model suggests that Brownian motion is crucial for demixing and that the non-diagonal elements of the collective diffusion tensor determines, which species enriches the center. Qualitative differences between 2 and 3 dimensions are found.

Finally, we present first results on monodisperse suspensions near close packing to understand flow oscillations and transient jamming.

[1] D. Semwogererea and E. R. Weeks, Phys. Fluids, 20, (2008).

[2] A. I. Campbell and M. D. Haw, Soft Matter 6, (2010).

CPP 1.8 Mon 11:30 C 130

**Rheological study of anisometric pigment particle suspensions** — •Yong Geng, Alexey Eremin, and Ralf Stannarius — Otto-von-Guericke-Universität Magdeburg, FNW/IEP/ANP, Postfach 4120, 39016 Magdeburg, Germany

Rheological properties of colloidal suspensions formed by nanometer size rod-shaped pigment particles dispersed in a non-polar solvent are studied. Experiments have shown that these suspensions possess unusual properties such as liquid crystalline behaviour at high dispersant concentration, field-induced phase separation at low and intermediate concentrations, switching in electric fields, and a reversible response to the adsorbing light affecting current transients in sandwich cells.1 By doping with small amounts of ferrofluid these pigment dispersions can form a basis for magneto-responsive materials. A strong magneto-optical effect has been confirmed. In our studies, we demonstrate a strong shear-induced birefringence and shear thinning behaviour in pure dispersions. We also discuss the effects of magnetic fields on the rheological properties of the pigment/ferrofluid mixtures. This helped to get a deeper insight into the properties of these suspensions and understand the mechanisms of the structural changes under external field such as electric, magnetic and flow.

1. Eremin, Alexey, et al., Adv. Funct. Materials 21.3 (2011): 556-564.

CPP 1.9 Mon 11:45 C 130

**Structure analysis of stable and metastable hard sphere fluids by confocal microscopy** — Achim Lederer[1] and •Hans Joachim Schöpe[2] — [1]Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, 55128 Mainz, Germany — [2]Eberhards Karls Universität Tübingen, Auf der Morgenstelle 10, 72026 Tübingen, Germany

The structural properties of the metastable melt play a key role in the understanding of the glass transition and crystal nucleation. Using laser scanning confocal microscopy we study the structure of stable and metastable colloidal hard sphere fluids. The used system was characterized with extreme care to allow a meaningful comparison with theory and simulation. While the Percus-Yevick (PY) approximation works quite perfectly for stable fluids at moderate volume fractions, it starts to fail for volume fractions larger than 0.45 approaching the freezing transition at 0.494. Strong deviation can be observed in metastable fluids: In the pair correlation function g(r) the experimental data display a significant higher principal peak and a different shape in the higher order peaks than the PY-approximation. In the static structure factor S(q) the data display a split in the second structure factor maximum suggesting a local short range crystalline like order. An analysis on the particle level reveals the existence of clusters with higher bond orientation order (q6(i)q6*(j)), although the overall hexagonal order of the ensemble does not increase.

CPP 1.10 Mon 12:00 C 130

**Effects of shear and walls on the diffusion of colloids in microchannels** — •somnath ghosh, frieder mugele, and michel duits — Physics of Complex Fluids group, MESA+ institute, University of Twente PO Box 217, 7500 AE Enschede, The Netherlands

Colloidal suspensions flowing through micro-channels were studied for the effects of both shear flow and the proximity of walls on the particles* self-diffusion. Use of hydrostatic pressure to pump micron-sized silica spheres dispersed in water-glycerol through poly (dimethylsiloxane) channels with a cross section of 30x24 micron, allowed variation of the Péclet number(Pé) from 0.01 to 50. To obtain diffusion coefficients, image-time series from a Confocal Scanning Laser Microscope were analysed with a method that, after finding the particle trajectories, subtracts the instantaneous convective displacements and subsequently measures the slopes of the Mean Squared Displacement in the flow (x) and shear (y) directions. The thus obtained Dx and Dy, which should be equal to the free diffusion coefficient (regardless of shear) in the dilute limit, both increase strongly with Péclet number (for Pé>10) in a concentrated suspension. This effect of shear-induced collisions is counteracted by the contribution of walls, which cause a strong local reduction in Dx and Dy.

CPP 1.11 Mon 12:15 C 130

**Transport of active particles in low-porosity structures** — Frank Wirner[1], Christian Scholz[1], and •Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universität Stuttgart, Germany — [2]Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany

Transport of active bacteria in porous media is of importance in many different fields, ranging from bioremediation, groundwater contamination and enhanced oil recovery to blood perfusion inside the body. We study the motion of active particles in artificially created porous media by a semi-experimental approach. In porous media with low porosities the presence of stagnant parts can lead to a temporary trapping of active particles in such regions, which can vastly increase their retention times. We compare the distributions of retention times and the transport properties of active and purely Brownian particles.

CPP 1.12 Mon 12:30 C 130

**Isobutyric acid and water mixture confined in a silica nanopore** — •Michael Harrach and Barbara Drossel — Institut für Festkörperphysik, TU Darmstadt, Darmstadt, Germany

We analyze the phase behaviour of water and isobutyric acid mixtures of differing weight percentages, in a silica nanopore of roughly 4 nm diameter and a corresponding smooth-walled confinement based on the average potential as given by the pore. While experimental studies have been interpreted as showing evidence for a phase seperation of water and isobutyric acid with the water situated at the pore wall we observe the converse, with the water rich part of the mixture preferring the pore center. The comparison of the smooth and rough pore allows us to further determine the importance of potential hydrogen bond sites and their influence on the static and dynamic characteristics of the mixture.

# CPP 2: Focus: Field Controllable Functional Polymers I

Time: Monday 9:30–12:30 Location: C 264

**Invited Talk** CPP 2.1 Mon 9:30 C 264

**Polymer films with optically controlled shape and functionality on a nanometer scale** — •Svetlana Santer — Universität Potsdam

When azo-modified photosensitive polymer films are irradiated with light interference patterns, topographic variations in the film develop that follow the field vector distribution resulting in the formation of surface relief gratings (SRG). In my talk I plan to address two major points concerning the experimental efforts to understand SRG formation in azobenzene containing thin polymer films: (i) how is the orientation of the electric field vector within the interfering electromagnetic fields related to the topographical pattern within the SRG; (ii) how can one measure locally the opto-mechanical forces emerging during topography change. In the first part, I will present a new set-up combining an atomic force microscope (AFM) and two-beam interferometry, with which it is possible to track the topography change in-situ while at the same time changing polarization and phase of the impinging interference pattern. In the second part of my talk I will present how graphene can be utilized as a nanoscopic probe in order to characterize local opto-mechanical forces generated within photosensitive azobenzene containing polymer films. Based upon our experimental results we can deduce that internal stresses within the film due to grating formation can exceed 1 GPa. To demonstrate the strength of the opto-mechanical forces generated within the polymer film in the last part of my talk I will report on opto-mechanical scission of polymer chains in photosensitive polymer brushes.

CPP 2.2 Mon 10:00 C 264

**Light-induced deformation of azobenzene-containing LC networks** — •Vladimir Toshchevikov[1], Tatiana Petrova[1,2], and Marina Saphiannikova[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V. — [2]Cherepovets State University, Russia

Azobenzene containing polymer networks belong to a class of smart materials, which are able to change their shape under light illumination. The photomechanical behavior of these materials is very sensitive to their chemical structure [1, 2]. In the present study we develop a theory of light-induced deformation of two-component polymer networks, which contain azobenzene chromophores and liquid crystalline (LC) mesogens. It is shown that preferential reorientation of chromophores perpendicular to the polarization direction leads to the reorientation of the mesogens due to LC interactions between the components. Reorientation of the chromophores and mesogens results in the light-induced deformation of the polymer network. The magnitude of deformation increases with increase of the volume fraction of chromophores and the strength of LC interactions between the components. Influence of the dilution of azobenzene networks by the bent cis-isomers of the chromophores on the light-induced deformation is discussed.

[1] V. Toshchevikov et al. J. Phys. Chem. B 116 (2012), 913; 118 (2014) 12297.

[2] V. Toshchevikov et al. J. Chem. Phys. 137 (2012), 024903.

CPP 2.3 Mon 10:15 C 264

**Towards Understanding Photoswitchable Materials: Molecular Dynamics Simulation Studies of Azobenzene-Containing Polymers** — •Marcus Böckmann and Nikos Doltsinis — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Münster, Germany

A large number of photoresponsive materials are made from polymers or liquid crystals that contain azobenzene (AB) as photochromic unit [1]. In this contribution, we will report on results from our theoretical studies based on multiscale molecular dynamics (MD) simulation techniques [2-4] applied to helical foldamers [4], artificial muscles [5], liquid crystals [3], and the phenomenon of photofluidity [6] yielding surface relief gratings (SRGs) in an active layer of poly-disperse-orange-3-metacrylamide (PDO3M).

[1] Y. Zhao and T. Ikeda, eds., *Smart Light-Responsive Materials: Azobenzene-ContainingPolymers and Liquid Crystals* (Wiley-VCH, Weinheim, 2009). [2] M. Böckmann, N. L. Doltsinis, and D. Marx, *J. Phys. Chem. A* **114**, 745 (2010). [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). [5] D. Bléger, T. Liebig, R. Thiermann, M. Maskos, J. P. Rabe, and S. Hecht *Angew. Chem. Int. Ed.* **50**, 12559 (2011). [6] P. Karageorgiev, D. Neher, B. Schulz, B. Stiller, U. Pietsch, M. Giersig, and L. Brehmer *Nature Materials* **4**, 699 (2005).

CPP 2.4 Mon 10:30 C 264

**Aggregation behaviour of doubly thermo-responsive poly(sulfobetaine-b-(N-isopropylmethacrylamide) diblock copolymers** — •Natalya Vishnevetskaya[1], Viet Hildebrand[2], Martine Philipp[1], André Laschewsky[2,3], Peter Müller-Buschbaum[1], and Christine Papadakis[1] — [1]TU München, Physik-Department, Physik weicher Materie — [2]Universität Potsdam, Institut für Chemie — [3]Fraunhofer Institut für Angewandte Polymerforschung IAP, Potsdam-Golm

Diblock copolymers consisting of non-ionic poly(N-isopropylmethacrylamide) (PNIPMAM block) and a zwitterionic poly(sulfobetaine) (PSB block) feature both a lower and an upper critical solution temperature (LCST and UCST) in aqueous solution. Accordingly, P(SB-b-NIPMAM)is expected to form (i) micelles with PNIPMAM shell and PSB core or vice versa at low and high temperatures and (ii) unimers or large aggregates in the intermediate temperature range, depending on the chemical structure and the molar mass of the PSB block as well as on the presence of electrolyte.

The phase transition temperatures in dependence on the electrolyte concentration are investigated via turbidimetry. The aggregation behavior modulated by dual stimuli (temperature and electrolyte concentration) is studied by temperature-resolved small-angle X-ray and neutron scattering (SAXS, SANS). Aggregation of P(SB-b-NIPMAM) in deuterated water was found to occur above LCST and below UCST. The structures formed depended markedly on the blocks lengths, whereas the salt-induced structural changes were only minor.

CPP 2.5 Mon 10:45 C 264

**Reversible thermosensitive biodegradable polymeric actuators driven by confined crystallization in thin films** — •Vladislav Stroganov and Leonid Ionov — Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Deutschland

Polymer actuators are materials capable of changing their shape in response to variation of environmental conditions, thus performing mechanical work. They have been used for many applications such as: controlling the liquid flow in microfluidical devices actuators, designing of swimmers, walkers, sensors, imaging devices, and 3D microfabrication. One of the promising fields of applications of polymeric actuators is the design of biomaterials such as stents, sutures as well as bio-scaffolds. For such kind of applications, polymeric actuators must be both biocompatible and biodegradable.

In this work we report design of biodegradable thermoresponsive polymeric films with reversible actuation based on polycaprolactone-gelatin bilayers. The films are unfolded at room temperature, fold at temperature above polycaprolactone melting point and unfold again at room temperature. The actuation is based on reversible switching of the structure of the hydrophobic polymer (polycaprolactone) upon melting and crystallization. We found that the origin of this completely unexpected behavior is the orientation of polycaprolactone chains parallel to the surface of the film, which is retained even after melting and crystallization of the polymer - *crystallization memory effect*. We also demonstrated potential application of such reversible biodegradable thermo-sensitive actuators for reversible encapsulation.

**15 min. break**

**Invited Talk** CPP 2.6 Mon 11:15 C 264

**Field Responses of Magnetic Gels** — Rudolf Weeber[1], Sofia S. Kantorovich[2], and •Christian Holm[1] — [1]Institut für Computerphysik, Universität Stuttgart, Stuttgart, Germany — [2]Universität Wien, Sensengasse 8, 1090 Wien, Austria

Ferrogels are hydrogels that additionally contain magnetic single-domain particles and whose properties can be controlled by using external magnetic fields. We will present recent results on the microstructure, the magnetic behavior, and the mechanical and viscoelastic properties of 2D and 3D magnetic gels on the basis of 2 microscopic particle models. In the first model the nano-magnets are part of the chain monomers, whereas in the second model the magnetic particles are restricted to the network nodes. We will focus on the magnetic field-actuated changes in the microstructure of the gel and correspondingly on the change in elastic behavior, magnetic response, and viscoelastic properties. We first summarize 2d computer models for the deformation by a change in the interaction between magnetic nano-particles [1]. Then we will present results for the second model where the deformation of the gel is triggered by torque transmission. In these systems, the polymer network is cross-linked by magnetic node particles. If time permits we will also present recent results on dipolar shifted particles [2].

[1] R. Weeber, S. Kantorovich, C. Holm, Soft Matter 8 (2012) 9923-9932. [2] R. Weeber, M. Klinkigt, S. Kantorovich, C. Holm, Journal of Chemical Physics 139 (2013) 214901.

CPP 2.7 Mon 11:45 C 264

**Electro-optics in fast switching polymer-stabilized liquid crystals of high chirality** — •Alexander Lorenz[1], Damian J. Gardiner[2], Rachel Hyman[2], Stephen M. Morris[3], and Timothy D. Wilkinson[2] — [1]Stranski-Laboratorium, Sek. TC 9, Technische Universität Berlin, Str. des 17. Juni 124, 10623 Berlin, Germany — [2]Centre of Molecular Materials for Photonics and Electronics, Department of Engineering, University of Cambridge, 9 JJ Thomson Avenue, Cambridge CB3 0FA, United Kingdom — [3]Department of Engineering Science University of Oxford, Parks Road, Oxford OX1 3PJ, United Kingdom

The electro-optic performance of a fast (< 1 ms) switching polymer-stabilized hyper-twisted chiral nematic LC [1] was rigorously analyzed with experiments and simulations: The induced birefringence was quantitatively traced back to both flexoelectro-optic switching and dielectric coupling [1]. In addition, a polymer-stabilized wide temperature blue phase LC [2] (based on well-known LC E7 and chiral dopant R5011) was generated in reflective test cells that possessed structured aluminum electrodes on a silicon wafer. A diffraction experiment revealed continuous, polarization independent optical phase modulation (maximum phase modulation depth of pi) in the thin (4 microns) polymer-stabilized LC layer [2]. 1. A. Lorenz et al., Applied Physics Letters 104, 071102 (2014). 2. R. M. Hyman et al., Applied Optics 53, 6925 (2014).

CPP 2.8 Mon 12:00 C 264

**Viscoelastic properties of magneto-sensitive elastomers** — •Dmytro Ivaneyko, Vladimir Toshchevikov, and Marina Saphiannikova — Leibniz-Institut für Polymerforschung Dresden e.V.

Magneto-sensitive elastomers (MSEs) are smart materials which consist of micron-sized magnetic particles dispersed within a non-magnetic elastomeric matrix. Mechanical properties of MSEs change considerably under external magnetic field [1]. In the present study we consider viscoelastic properties of isotropic MSEs using a coarse-grained cubic network model, which describes the network dynamics in the low-frequency regime [2]. Equations of motion for magnetic particles take into account topology of the elastic network and magnetic interactions between the particles. We show that the application of uniform magnetic field leads to the splitting of the relaxation spectrum into two branches for the motions of the particles parallel and perpendicular to the field. The shear dynamic moduli G' and G" of MSEs are calculated as functions of the frequency. The values of G' and G" are shown to depend on the direction of the shear deformation with respect to the magnetic field. For instance, both G' and G" increase if the shear is applied perpendicular to the direction of the magnetic field. This prediction is in a qualitative agreement with existing experimental data.

[1] D. Ivaneyko et al., Soft Matter 10 (2014), 2213.

[2] V.P. Toshchevikov et al., Macromolecules 42 (2009), 3417.

CPP 2.9 Mon 12:15 C 264

**Mesoscopic modeling of ferrogels and magnetic elastomers** — Peet Cremer[1], Giorgio Pessot[1], Mitsusuke Tarama[1,2], Elshad Allahyarov[1], Hartmut Löwen[1], and •Andreas M. Menzel[1] — [1]Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany — [2]Kyoto University, Kyoto, Japan

Ferrogels and magnetic elastomers consist of colloidal magnetic particles embedded in a crosslinked polymer matrix. Tunable elastic moduli that can be switched by an external magnetic field represent one of their outstanding features. Our goal is to understand and identify such controllable material properties on the magnetic particle level using both particle-matrix and simplified dipole-spring models.

We studied how the particle arrangement and orientation of the magnetic moments can influence the elastic moduli when the strength of the magnetic interaction is controlled. In one case, we used the particle distribution of a real experimental sample as an input. Here, the convenient technical assumption of affine deformations must be dropped. Furthermore, we demonstrated that the relaxation dynamics of the materials can be tuned by the particle arrangement, by external magnetic fields, and by an orientational memory. Apart from that we showed that a pronounced switchable nonlinear stress-strain behavior is found under suitable circumstances.

In the future, we aim at a connection of our characterization to more microscopic and to macroscopic scales. We have already taken the first steps into these directions by comparing to minimum Monte-Carlo simulations and by performing a simplified coarse-graining procedure.

## CPP 3: Nanoparticles and Composite Materials I (joint session CPP, BP)

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

CPP 3.1 Mon 9:30 C 243

**Iron Oxide Nancube Monolayers at the Air/Water Interface: Self-Organization on Nano- and Mikroscale** — •Heiko Ahrens[1], Sarah Mehdizadeh Taheri[2], Thomas Ortmann[1], Andreas Gröning[1], Stephan Förster[2], and Christiane A. Helm[1] — [1]Physik, Uni Greifswald, 17487 Greifswald, Germany — [2]Physikalische Chemie I, Uni Bayreuth, 95440 Bayreuth, Germany

Monodisperse Cubic Iron Oxide nano particles (5-8 nm) covered in oleic acid form stable films on the air water interface. Isotherms exhibit a plateau at 18 - 20 mN/m, then the pressure increases steeply. At zero surface pressure, Brewster angle microscopy(BAM)shows micrometer sized domains consisting of nanocubes immersed in a matrix of excess oleic acid. These small domains show Brownian motion. Then linear and mesh-like rigid domains (size 100 *m) are observed. The 5.5nm nanocubes form a homogenous monolayer in the plateau region, on further pressure increase large (100 *m) homogenous domains of bi- and even multilayer appear. The films of the larger 8 nm nanocubes remain heterogeneous at all surface pressures. Large (100 *m) patches of oleic acid monolayers coexist with medium sized (50*m) domains of particle monolayer and small domains (10 *m) of bi- and multilayers. All aggregation is irreversible.

These observations are confirmed by X-ray reflectivity and Grazing Incidence X-ray diffraction.

CPP 3.2 Mon 9:45 C 243

**ZnO nanoparticle stabilization - How much is necessary?** — •Torben Schindler[1], Tilo Schmutzler[1], Wei Lin[2], Doris Segets[2], Wolfgang Peukert[2], and Tobias Unruh[1] — [1]Lehrstuhl für Kristallographie und Strukturphysik, Friedrich-Alexander-Universität Erlangen Nürnberg, Staudtstr. 3, 91058 Erlangen — [2]Lehrstuhl für Feststoff- und Grenzflächenverfahrenstechnik, Friedrich-Alexander-Universität Erlangen Nürnberg, Cauerstr. 4, 91058 Erlangen

The stabilization of small nanoparticles is of highest importance for their use in different applications. For these applications the stabilizer used in the synthesis is often exchanged by different species which offer the possibility of e.g. light harvesting for solar cells. However, the amount of stabilizer needed in the first place was seldomly addressed in the literature. In the case of solution processed ZnO nanoparticles acetate is often used as primary stabilizer. However, by washing of the samples it was observed that the nanoparticles become unstable and show strong agglomeration after three washing cycles. We investigated the changes in the stabilizing acetate layer by the combination of small angle X-ray and neutron scattering (SAXS&SANS). Initially the shell incorporates about 10% of the total acetate. This factor is clearly reduced in the washed samples which show still stability against agglomeration. Thus only a small amount of acetate is actually needed to stabilize the nanoparticles. In addition to these results the effect of first ligand exchange reactions using different amounts of catechol will be presented.

CPP 3.3 Mon 10:00 C 243

**A Toolbox to Connect the Physicochemical Properties of GNPs with their Biological Behavior** — •Jonas Schubert and Munish Chanana — Department of Physical Chemistry II, University of Bayreuth, 95440 Bayreuth (Germany)

Due to their plasmonic properties and their biocompatibility gold nanoparticles (GNPs) are widely used in biological systems. Unfortunately, the colloidal variability is neglected in most studies, so that the chemical identity is not coherent with the biological identity. An undefined absorption alters the properties of the particles fundamentally, so that it is not possible to predict or study their biological behavior in dependence of their original physicochemical properties, e.g. surface charge.

To circumvent these problems, we present a toolbox of GNPs with a defined protein corona.[1,2] This defined protein corona enables the GNPs to meet the first requirement for biological applications: high colloidal stability in the presence of salt, other proteins and over a large range of pH values. A toolbox of more than 10 proteins and different purification procedures allow the exceptional chance of tailoring the physicochemical properties of nanoparticles, such as surface charge, colloidal stability and responsiveness.

1Chanana, M.; Correa-Duarte, M. A.; Liz-Marzan, L. M., Small 2011, 7 (18), 2650-2660.

2Chanana, M.; Gil, P. R.; Correa-Duarte, M. A.; Liz-Marzan, L. M.; Parak, W. J., Angewandte Chemie-International Edition 2013, 52 (15), 4179-4183.

CPP 3.4 Mon 10:15 C 243

**Electrochemical growth of ZnO nanostructures for biosensing applications** — •Raluca - Ancuta Suciu, Nivedita Yumnam, and Veit Wagner — Jacobs University, Bremen, Germany

Biosensors have been used in applications such as blood glucose measuring or pregnancy tests already for a long time, and their improvement is of high interest in many fields of research such as medicine (e.g. diagnostics), military (e.g. monitoring of poison gases) and industry (e.g. food and drink process control). The sensitivity of biosensors can be improved by increasing the surface area where the molecules under observation can bind. Therefore, we have employed ZnO nanorods grown via electrochemical deposition on Au covered flexible PET (polyethylene terepthalate) substrate. The size and distance of ZnO nanostructures can be effectively controlled by tuning the electrochemical deposition parameters. Furthermore, self-assembled monolayer (SAM) of 1-octadecanethiol has been applied on Au to tune the nucleation density of ZnO. Application of SAM prevents overly dense growth of ZnO and instead allows ZnO to electrochemically grow through the pinholes in the SAM. To realize a capacitive sensor additional Au finger contacts have been fabricated using optical lithography. The sensor operation is verified by detection of Streptavidine biomolecules.

CPP 3.5 Mon 10:30 C 243

**In situ Study of Spray-deposited Gold Nanoparticles Assemblies on Polymer Substrates Using GISAXS** — •Peng Zhang[1], Koyiloth v. Sarathlal[1], Santoro Gonzalo[1], Nipam Shah[2], Guangsu Huang[3], and Stephan v. Roth[1] — [1]Deutsches Elektronen Synchrotron, Notkestr. 85,22607 Hamburg — [2]Fachbereichs Maschinenbau und Wirtschaft, Fachhochschule Lübeck, 23562 Lübeck — [3]College of Polymer Science and Engineering, State Key Laboratory of Polymer Materials Engineering, Sichuan University, Chengdu 610065, China

The assembly of the nanoparticles from the solution still remains challenging, namely inhomogeneous material dispersion for example, coffee-stain-like or clumps of particles is observed1. To get designed nanocomposite in thin films, controlling the solution evaporation and promoting the ordering of nanoparticles on the templated substrates is a smart and feasible choice. Spray deposition is one of the desirable techniques to manipulate solvent evaporation by atomizing the solution2,3. Here we present our recent in situ studies on the directed assembly of spray deposited gold nanoparticles on patterned substrates. By manipulating the assembly process, we find that the well-ordered gold nanoparticles show enhanced optical properties. These findings are attractive for the applications such as solar cells and antireflection coating. [1] Yunker et al. Nature 476, 308 (2011); [2] Al-Hussein et al. Langmuir 29, 2490 (2013); [3]Herzog et al. Langmuir 29, 11260 (2013).

**Invited Talk** CPP 3.6 Mon 10:45 C 243

**Functional Nanocomposites: Disordered media with a cooperative macroscopic action** — •Mady Elbahri — Nanochemistry and Nanoengineering, Institute for Materials Science,Faculty of Engineering, Christian-Albrechts-University Kiel, Germany

So far, research on polymer based nanocomposites mostly centered on structural composites where little attempt was made to precisely control the nanostructure. During the last years, however, there has been increasing interest in functional nanocomposites due to novel applications ranging from sensors and plasmonics through stretchable electronics and smart coatings to energy conversion and human health. In this context the concept of a disordered "glassy" nanocomposite with a cooperative macroscopic action has not been suggested so far. The present talk aims at introducing a particularly promising new class of functional optical materials based on closely spaced ultrafine nanoparticles acting as "artificial molecules" embedded in a polymeric host where the unique properties arise from the strong and cooperative near field coupling between neighbouring nanoparticles. This gives rise to coherent cooperative action thus determining the macroscopic properties.

**15 min. break**

CPP 3.7 Mon 11:30 C 243

**Self-assembly of nanoparticles in block copolymer nanotemplates** — •Manfred Stamm[1,2], Andreij Horechyy[1], and Bhandu Nandan[3] — [1]Leibniz-Institut für Polymerforschung Dresden — [2]Technische Universität Dresden — [3]Indian Institute of Technology, Delhi

Nanotemplates generated by microphase segregation of diblock copolymers can be used for directed self-assembly of nanoparticles. There are several routes possible where functional nanoparticles are either added to the copolymer solution prior to film formation and then preferentially migrate to one of the phases or where the nanoparticles are added after copolymer nanotemplate formation and then show preferential adsorption to one of the phases. In both cases ordered nanoparticle arrays are obtained and by combination of the two approaches dual structures /1/ may be formed. With hexagonal structures and removal of the majority phase, nanorods are generated /2/. Under certain conditions helical arrangements of nanoparticles inside the cylinders are observed /3/ which are due to dense packing in confined geometry. Copolymer nanotemplates thus provide an interesting tool for generation of ordered nanoparticle structures. We acknowledge funding by DFG. /1/ Adv.Fun.Mater. 23 (2013) 483-90; /2/ J.Mater.Chem. 22 (2012) 25102-7; /3/ Angew. Chem. Int. Ed. 53 (2014) 1-5.

CPP 3.8 Mon 11:45 C 243

**Insulin capped gold nanoparticles-polymer brush composites** — •Muriel Rovira Esteva, Zuleyha Yenice, Stephanie Christau, Stefan Wellert, and Regine von Klitzing — Stranski Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, 10623 Berlin, Germany

Polymer brushes are polymers grafted to a surface by one end, with a density high enough to induce the polymer chains to stretch away from the surface. This stretching is often responsive to environmental conditions, which makes them a suitable candidate for the design of smart coatings, among a number of other applications. Polymer brush-nanoparticle composites allow to combine the responsive properties of the brush with the physico-chemical properties of the particles. Therefore, determination of how the geometric parameters affect the behavior of the composite is of high scientific and technological significance.

Gold nanoparticles capped with sodium citrate are often used in these composites, but they pose a series of instability problems. In this work, monodisperse gold nanoparticles with sodium citrate and tannic acid cappings were synthesized, and their capping was replaced by insulin, adapting a method by M. Chanana et al. The higher stability against strong pH variations of the insulin capped particles was confirmed with UV-Vis. Incorporation of particles with different cappings into brushes with different geometries allowed to obtain a variety of polymer brush-gold nanoparticle composites, and the effect of the geometrical parameters on the brush-nanoparticle interactions was then explored using a number of techniques, such as AFM and reflectometry.

CPP 3.9 Mon 12:00 C 243

**Drug delivery to cancer cells by nanodiamonds** — •Anna Ermakova[1], Yuzhou Wu[2], Boris Naydenov[1], Tanja Weil[2], and Fedor Jelezko[1] — [1]Institute of Quantum Optics, University Ulm, Ulm, Germany — [2]Institute of Organic Chemistry III, University Ulm, Ulm, Germany

The numbers of new cancer cases increase every year, and only few last years in some country the numbers of deaths were stable or decreased [1], this is result of progress in medicine. The main problem of the cancer therapy is the precise drug delivery to cancer cells with the exception of healthy cells. The direct drug delivery can bring a lot of advantages: reduction of the total amount of uptaken drug, more stable drug level in the specific sides, potential reduction of the drug in healthy unaffected tissues, and reduction of dosages frequency. Nanodiamonds (NDs) are potentially good drug carriers since they are non-toxic [2], their surfaces can be chemically functionalized [3] and they can be easily inserted into cells [4]. Furthermore, colour defect centres in NDs can be used as photostable biomarkers compared to quantum dots and dyes. In our work to release drug we used the property of the tumour tissue to have on average a lower pH level than healthy tissue [5]. We demonstrate a drug release from NDs in the solution, triggered by change in the pH, and inside HeLa cells. We show that only drugs penetrate into a cell nucleus and NDs stay at the cytoplasm. [1]R.Siegel et al,CA Cancer J Clin,63(2013) [2]A.M.Schrand et al,J Phys Chem B,111(2007) [3]A.Datta et al.,Nanotechnology,22(2011) [4]F.Neugart et al.,NanoLett.,7(2007) [5]R.Jain,J of Controlled Release,53(1998)

CPP 3.10 Mon 12:15 C 243

**Metal nanopattering using block copolymers: Differences between ionic and atomic metal selectivity** — •Ezzeldin Metwalli[1], Yuan Yao[1], Volker Körstgens[1], Matthias Schwartzkopf[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]DESY, Notkestr. 85, 22607 Hamburg

Metal nano-patterns with a particular structural symmetry, characteristic length scale and periodicity are of growing interest, e.g. for photonic applications and high-density memory devices. The characteristic metal affinity towards the minority block of the self-assembled block copolymer (BC) templates plays an essential role to fabricate highly-order and well-defined metal nanopatterns [1]. Though, ions of metal are highly selective towards the ionic polymer block, the metal atoms show an opposite behavior, an extreme selectivity towards the neutral block. A simple explanation based on like-dissolves-like is ruled out. Experiments are performed by depositing gold in its atomic state on several homopolymer and block copolymer films with DC magnetron sputtering. At time resolution of 15 milliseconds, the nucleation/growth kinetics of gold nanoparticles on the polymer films is monitored using in-situ GISAXS. An extreme selectivity of the metal atoms is observed on the neutral block with an exponential growth of metal particle size. The coalescence behavior of the inert metal is mainly dominated by the improved atom mobility within the neutral polymer block. [1] Metwalli et al. ChemPhysChem 15, 2236 (2014)

CPP 3.11 Mon 12:30 C 243

**Nanocomposites of colloidal triglyceride platelets and DNA** — •Martin Schmiele, Charlotte Knittel, and Tobias Unruh — Physik Department, Friedrich-Alexander-Universität Erlangen–Nürnberg, Staudtstr. 3, 91058 Erlangen, Germany

Aqueous suspensions of colloidal tripalmitin platelets, stabilized by a mixture of soybean lecithin, Poloxamer 188 (or Polysorbate 80) and the cationic surfactant dioctadecyldimethylammonium bromide (DODAB), are prepared by high-pressure melt homogenization. DODAB provides the platelets with a positive surface charge. DNA complexes are prepared by addition of herring DNA to the suspensions.

The structure of the DNA complexes, ranging from the molecular to the micron scale, is investigated by small- and wide-angle x-ray and neutron scattering, microcalorimetry, photon correlation spectroscopy, transmission electron microscopy and computer simulations.

Complexes prepared from native suspensions with low concentrations of DODAB and high +/− charge ratios (DODAB:DNA) exhibit sizes in the colloidal range. Higher concentrations of DODAB and charge ratios close to the isoelectric point promote platelet agglomeration, leading to very large complexes of several microns.

Small-angle scattering and computer simulations reveal a lamellar arrangement of the platelets in the complexes, with the DNA being most probably sandwiched between the platelets. Such nanocomposites of macromolecules (DNA) and tripalmitin platelets could provide a good protection of the intercalated macromolecules and can be regarded as a potential carrier system for them.

CPP 3.12 Mon 12:45 C 243

**Nanocomposites composed of HEUR polymer and magnetite iron oxide nanoparticles** — •Antonella Campanella[1], Henrich Frielinghaus[1], Zhenyu Di[1], Marie-Sousai Appavou[1], Alessandra Luchini[2], Luigi Paduano[2], Alice Klapper[3], Oleg Petracic[3], Peter Müller-Buschbaum[4], and Dieter Richter[1] — [1]JCNS@FRMII, Lichtenbergstrasse 1, 85747 Garching — [2]University of Naples, Federico II, Dipartimento di Scienze Chimiche, Via Cinthia, 80126 Naples,Italy — [3]JCNS-2, Forschungszentrum Jülich GmbH, 52425 Jülich — [4]TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Strasse 1, 85748 Garching

We study nanocomposites of a polymer matrix which consists of hydrophobically modified ethoxylated urethane polymers (HEUR) with embedded coated magnetite nanoparticles. Two different kinds of coatings are compared namely, the hydrophobic coating, composed of oleic acid and oleylamine, and the hydrophilic coating composed of a cationic surfactant, C18TAB, as an additional layer to the hydrophobic magnetic nanoparticles. We focused on the structural characterization of such nanocomposites in two different morphologies: as thin dry films and as hydrogels.

## CPP 4: Statistical Physics in Biological Systems (joint session DY, BP, CPP)

Time: Monday 9:30–12:15 Location: BH-N 243

**Invited Talk** CPP 4.1 Mon 9:30 BH-N 243

**Chemical warfare and survival strategies in bacterial range expansions** — Markus F Weber, Gabriele Poxleitner, Elke Hebisch, Erwin Frey, and •Madeleine Opitz — Center for NanoScience, Faculty of Physics, Ludwig-Maximilians-Universität München, Munich, Germany

Spreading of species into uncolonized territory is a fundamental ecological process in the evolution and maintenance of biological diversity. Although interactions between species have experimentally been identified as major determinants of species coexistence in spatially extended populations, their role in spatially expanding populations is largely unknown. Here, we address the roles of resource and interference competition by genetically tuning a bacterial model system of three Escherichia coli strains: a toxin (colicin) producing strain, a sensitive strain, and a resistant strain. We show that maintenance of biodiversity is determined by three strongly interdependent ecological factors: the relative ratio of the competing strains, their growth rates and the strength of toxicity. Our mathematical analysis suggests, that despite general expectations, a non-hierarchical interaction network is not a necessary prerequisite for biological diversity. Moreover, we find that robust three-strain coexistence requires a balance between growth rates and a small enough toxicity range or, alternatively, a reduced initial ratio of the colicin-producing strain. We expect that the approach presented in this study will be useful to identify further mechanisms for the maintenance of biodiversity in microbial communities.

CPP 4.2 Mon 10:00 BH-N 243

**A New Dimension: The Influence of Two Dimensional Niche Space on Evolutionary Food Web Models** — •Daniel Ritterskamp and Bernd Blasius — ICBM, University Oldenburg, Germany

Food webs encode feeding interactions of ecological communities, originating from an intricate interplay of evolutionary and ecological processes. This dynamic can be described by evolutionary food web models, in which feeding interactions between species are related to the relative distance of their adaptive traits (e.g., body size) on a niche axis. However, not much is known about evolutionary food web dynamics in space.

Here, we go beyond traditional approaches and develop an evolutionary food web model in a two dimensional niche space, where the additional niche axis might describe a spatial coordinate or an environmental variable. Using numerical simulations, we investigate population dynamics, evolutionary behaviour and the emerging community structure in space. The model is able to produce both static and dynamic food webs, depending on the width of the interaction kernel; whereas food web complexity is determined mainly by the interaction strength.

We observe rich dynamics including: spatio-temporal patterns, arms races, red queen dynamics, as well as sub-food webs moving in space. By sampling the spatial axis, local food webs are recovered, which can be related to empirical data. We conclude that the additional niche-dimension is essential to capture realistic patterns of spatially structured food webs.

CPP 4.3 Mon 10:15 BH-N 243

**Biodiversity and ecosystem functioning in evolving food webs** — •Korinna T. Allhoff and Barbara Drossel — TU Darmstadt, Germany

We analyze an evolutionary food web model where each species is characterized by three traits, namely its own body mass, its preferred prey body mass, and the width of its potential prey body mass spectrum. Population dynamics includes feeding and competition interactions and determines which species are viable and which ones go extinct. On a timescale much slower than population dynamics, new species emerge as modifications of existing species. The network structure emerges according to the interplay between population dynamics and evolutionary rules and shows an ongoing species turnover. The model thus gives insights into how the functional diversity changes during the initial network buildup as well as due to extinction avalanches. We investigate the relation between the functional diversity and five community level measures of ecosystem functioning. These are the metabolic loss of the predator community, the total biomasses of the basal and the predator community and the consumption rates on the basal community and within the predator community.

CPP 4.4 Mon 10:30 BH-N 243

**Efficiency of cellular information processing** — •David Hartich, Andre C. Barato, and Udo Seifert — II. Institut für Theoretische Physik, Stuttgart, Germany

We study theoretical models inspired by the *E. coli* sensory network, using the framework of stochastic thermodynamics for bipartite systems [1]. More precisely, we model the sensory system by an internal process measuring an external process, which is a ligand concentration jumping at random between two values. We show that the rate of conditional Shannon entropy reduction, characterizing the learning of the internal process about the external process, is bound by the thermodynamic entropy production [2]. This approach allows for the definition of an informational efficiency that can be used to study cellular information processing. We start with a simple model for which ATP must be consumed so that a protein inside the cell can learn about the external environment. A further discussion illustrates, *inter alia*, that a non-zero learning rate without dissipation inside the cell can only be obtained if the external process compensates for it.

[1] DH, ACB and US, J. Stat. Mech., P02016 (2014)

[2] ACB, DH and US, New J. Phys. **16**, 103024 (2014)

CPP 4.5 Mon 10:45 BH-N 243

**Tackling your free energy estimates with pyfeat** — •Antonia Mey, Christoph Wehmeyer, Fabian Paul, Hao Wu, and Frank Noé — Institut für Mathematik, FU Berlin

Understanding the equilibrium properties of physical systems is of general interest in many different areas of physics. In complex systems, equilibrium properties can often only be evaluated by means of numerical simulations, which are frequently plagued by rare event dynamics. One approach to circumvent rare event dynamics is to use enhanced sampling methods (e.g. replica exchange methods or umbrella sampling).

The range of established analysis methods to optimally estimate equilibrium properties from multi-ensemble simulations often requires an expert user for their implementation or even usage. Here, we introduce a new software package, the python free energy analysis toolkit – pyfeat, that facilitates the analysis of multi-ensemble simulation. Pyfeat provides an easy-to-use interface to well established methods such as WHAM or MBAR, as well as the recently introduced transition-based reweighting analysis methods (TRAM), which borrow ideas from Markov state models. The software's straight forward usability makes comparing different estimation method applied to the same input data trivial.

Generally, any multi-ensemble simulation can be used for the analysis ranging from all-atom protein molecular dynamics simulations to simulations of condensed matter systems. Pyfeat is available for download at: https://github.com/markovmodel/pyfeat.

**15 min. break**

CPP 4.6 Mon 11:15 BH-N 243

**Lateral domain formation in membranes coupled to curvature** — •Sina Sadeghi, Marcus Müller, and Richard Vink — Institute of Theoretical Physics, Georg-August-Universität Göttingen, Göttingen, Germany

The lateral heterogeneity in the plasma membrane of eukaryotic cells is an important factor for regulating biological functions. As opposed to plasma membranes, model membranes (either artificially prepared membranes, or membranes extracted from living cells) typically phase separate. To address this paradox, we present computer simulations of a coarse-grained membrane model that undergoes macroscopic phase separation at low temperature. Considering a coupling between local composition and local curvature of the membrane, we show that the system exhibits composition fluctuations with a nontrivial length scale, resembling microemulsion. The latter is identified as a region where lipid rafts can form. We furthermore probe the nature of phase transition between the phase-separating regime and the mixed state. This transition is continuous and belongs to the two-dimensional Ising universality class for weak coupling to curvature, but becomes first-order for strong curvature-composition coupling.

CPP 4.7 Mon 11:30 BH-N 243

**DNA denaturation transition: environmental effects on scaling** — •Christian von Ferber[1] and Yurij Holovatch[2] — [1]Coventry University, UK — [2]Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, Lviv, UA

The Poland and Scheraga model for the DNA denaturation transition is reconsidered taking into account environmental effects. We apply field theoretical methods to discuss environmental effects on the nature of the transition. In particular we discuss variants of the transition that may occur due to particular properties of the environment. These are the presence of uncorrelated and power-law long-range correlated disorder which influences the transition as function of the power law exponent, the quality of the solution which may affect the self- and mutual interaction of both single and double strands and combination of these. All these have significant effects on the transition.

CPP 4.8 Mon 11:45 BH-N 243

**Variational approach to molecular dynamics** — •Bettina Keller — Freie Universität Berlin, Institut für Chemie und Biochemie, Takustraße 3, 14195 Berlin

The eigenvalues and eigenfunctions of the classical molecular dynamics propagator contain the essential information about the molecular thermodynamics and kinetics. A matrix representation of the propagator can be constructed by partitioning the conformational space into discrete states and estimating the state-to-state transition probabilities from molecular dynamics simulations, yielding a so-called Markov state model (MSM). The precision of an MSM depends sensitively on on how well the discretization reproduces the shape of the dominant eigenfunctions. The difficulty to find a suitable discretization has limited the routine use of MSMs. Moreover, most discretizations are data-driven, impairing the comparison between MSMs and the interpretation of the eigenvectors in terms of structural transitions.

Using a recently published variational approach, it is possible to construct a matrix representation of the propagator using an arbitrary basis set, allowing to use basis functions with gentle slopes. This reduces the discretization error. More importantly, the user can define basis sets which have a chemical meaning and can be used for entire classes of molecules, thereby allowing for direct comparison of the kinetic models. I will give an overview of the variational principle for the classical molecular dynamics propagator and propose a basis set for peptide dynamics which is based on the dominant eigenfunctions of individual amino acids

CPP 4.9 Mon 12:00 BH-N 243

**Simple association-dissociation-aging process: recursive solution** — •Thomas Niedermayer and Reinhard Lipowsky — Max

Planck Institute of Colloids and Interfaces, Potsdam, Germany

The simple association-dissociation-aging process (SADAP) is characterized by the coupling of stochastic growth and shrinkage of one-dimensional structures to the random aging of the constituting subunits. Most prominently, SADAPs capture the essential features of the polymerization of actin filaments and microtubules. Previously employed mean field methods fail to describe the dynamics of SADAPs. We found an ansatz for the full master equation which allows us to study SADAPs analytically and derive a recursion relation for the steady state solution which enables the calculation of all emergent quantities with increasing accuracy. In particular, our method allows, for the first time, the precise calculation of the boundary between the growth and shrinkage regime, in excellent agreement with results from stochastic simulations.

## CPP 5: Anomalous Diffusion (joint session DY, CPP)

Time: Monday 9:30–12:00 Location: BH-N 334

CPP 5.1 Mon 9:30 BH-N 334

**Anomalous diffusion in corrugated potentials with spatial correlations: faster than normal, and other surprises** — •Igor Goychuk — Institute for Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24/25, 14476 Potsdam-Golm, Germany

Normal diffusion in corrugated potentials with spatially uncorrelated Gaussian energy disorder famously explains the origin of non-Arrhenius $\exp[-\sigma^2/(k_BT)^2]$ temperature-dependence in disordered systems. We show [1] that unbiased diffusion remains asymptotically normal also in the presence of spatial correlations decaying to zero. However, due to a temporal lack of self-averaging transient subdiffusion emerges on mesoscale, and it can readily reach macroscale even for moderately strong disorder fluctuations of $\sigma \sim 4 - 5\,k_BT$. Due to its nonergodic origin such subdiffusion exhibits a large scatter in single trajectory averages. However, at odds with intuition, it occurs essentially faster than one expects from the normal diffusion in the absence of correlations. We apply these results to diffusion of regulatory proteins on DNA molecules and predict that such diffusion should be anomalous, but much faster than earlier expected on a typical length of genes for a realistic energy disorder of several room $k_BT$, or merely 0.05 – 0.075 eV.

[1] I. Goychuk and V. Kharchenko, Phys. Rev. Lett. **113**, 100601 (2014).

CPP 5.2 Mon 9:45 BH-N 334

**Path Probabilities of Continuous Time Random Walks** — •Stephan Eule — MPI fuer Dynamik und Selbstorganisation

Employing the path integral formulation of a broad class of anomalous diffusion processes, we derive exact relations for path probability densities of these processes. In particular, we obtain a closed analytical solution for the path probability distribution of a Continuous Time Random Walk (CTRW) process. This solution is given in terms of its waiting time distribution and short time propagator of the corresponding random walk as a solution of a Dyson equation. Applying our analytical solution we derive generalized Feynman-Kac formulae.

CPP 5.3 Mon 10:00 BH-N 334

**Nonergodicity in scaled Brownian motion** — •Felix Thiel and Igor M. Sokolov — Institut für Physik der Humboldt Universität zu Berlin: Newtonstraße 15, 12489 Berlin, Deutschland

Scaled Brownian motion (sBm) is a random process described by a diffusion equation with explicitly time-dependent diffusion coefficient (Batchelor's equation), which is often used for fitting experimental data for subdiffusion of unclear genesis. We show that it describes the rescaled mean position of a cloud of independent continuous time random walkers. Like the latter, sBm is neither stationary nor ergodic. Unlike continuous time random walks, the nonergodicity of sBm is not accompanied by a strong difference between its different realizations: its heterogeneity ("ergodicity breaking") parameter tends to zero for long trajectories.

CPP 5.4 Mon 10:15 BH-N 334

**Understanding and Controlling Regime Switching in Molecular Diffusion** — •Sarah Hallerberg[1] and Astrid S. de Wijn[2] — [1]Network Dynamics, Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen — [2]Department of Physics, Stockholm University

Diffusion can be strongly affected by ballistic flights (long jumps) as well as long-lived sticking trajectories (long sticks). Using statistical inference techniques in the spirit of Granger causality, we investigate the appearance of long jumps and sticks in molecular-dynamics simulations of diffusion in a prototype system, a benzene molecule on a graphite substrate. We find that specific fluctuations in certain, but not all, internal degrees of freedom of the molecule can be linked to either long jumps or sticks. Furthermore, by changing the prevalence of these predictors with an outside influence, the diffusion of the molecule can be controlled. The approach presented in this proof of concept study is very generic, and can be applied to larger and more complex molecules. Additionally, the predictor variables can be chosen in a general way so as to be accessible in experiments, making the method feasible for control of diffusion in applications. Our results also demonstrate that data-mining techniques can be used to investigate the phase-space structure of high-dimensional nonlinear dynamical systems.

Phys. Rev. E 90, 062901, 2014

CPP 5.5 Mon 10:30 BH-N 334

**Optimisation of search efficiency by combination of Levy flights and Brownian motion** — •Vladimir V. Palyulin — Physics Department, Technical University of Munich, D-85747 Garching, Germany

Problems of target search occur in a wide range of applications ranging from animals looking for prey to diffusion control of molecular processes. For a long time the field was dominated before by a notion, that Lévy flights with a critical exponent $\alpha = 1$ are optimal. Recently we proved that this statement is not always correct, and often Brownian motion presents a better alternative [1]. In this new study we show that intermittent search, which consists of Lévy flights and Brownian motion presents even better alternative. In order to show that we computed an average of inverse rate of target location, which works as a good measure of search efficiency. Analytical and numerical results are obtained from fractional Fokker-Planck equation and supported by Monte-Carlo simulations.

[1] V.V. Palyulin, A.V. Chechkin and R. Metzler, Proc. Natl. Acad. Sci. USA, **111**, 2931 (2014).

**15 min. break**

CPP 5.6 Mon 11:00 BH-N 334

**Single-file diffusion in a quenched energy landscape** — •Henning Krüsemann[1] and Ralf Metzler[1,2] — [1]University of Potsdam, Potsdam, Germany — [2]Tampere University of Technology, Tampere, Finland

The diffusion of hardcore interacting particles in a narrow (1D) channel is called single-file diffusion. Examples in physics can be found especially in biophysics, e.g. the transport of molecules through a narrow pore.

The dynamical properties in a single file differ strongly from those of freely diffusing particles and different types of subdiffusion can be observed.

In this talk we discuss the msd of single-file diffusion with different particle interactions in a quenched energy landscape. We present simulation results and approach the problem theoretically.

CPP 5.7 Mon 11:15 BH-N 334

**Dynamical consequences of oriented particles interacting with their fractal surrounding** — •Janett Prehl[1], René Haber[1], Heiko Herrmann[1,2], and Karl Heinz Hoffmann[1] — [1]Institut für Physik, Technische Universiät Chemnitz, Chemnitz, Deutschland — [2]Centre for Nonlinear Studies, Tallinn University of Technology, Tallinn, Estland

In order to model diffusive particles in porous media, often random walks of point particles on fractals are utilized as model system. It exhibits subdiffusive behavior, where the anomalous diffusion exponent is smaller than one, and the corresponding random walk dimension is larger than two. This is due to the limited space available in fractal structures. Within this presentation we endow the particles with an orientation [1, 2] and analyze their dynamics on fractal structures. In particular, we focus on the dynamical consequences of the interactions between the local surrounding fractal structure and the particle orientation, which are modeled using an appropriate move class. These interactions can lead to particles becoming temporarily or permanently stuck in parts of the structure. A surprising finding is that the random walk dimension is not affected by the orientation while the diffusion constant shows a variety of interesting and surprising features.

[1] R. Haber, J. Prehl, K. H. Hoffmann, and Heiko Herrmann, *J. Phys. A: Math. Theor.* **47** (2014) 155001
[2] R. Haber, J. Prehl, H. Herrmann, and K. H. Hoffmann, *Phys. Lett. A* **377** (2013) 2840–2845

CPP 5.8 Mon 11:30 BH-N 334

**Fractal grid comb model** — •Trifce Sandev[1,2], Alexander Iomin[2,3], and Holger Kantz[2] — [1]Radiation Safety Directorate, Partizanski odredi 143, P.O. Box 22, 1020 Skopje, Macedonia — [2]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, 01187 Dresden, Germany — [3]Department of Physics, Technion, Haifa 32000, Israel

A grid comb model is a generalization of the well known comb model, and it consists of N backbones. For N=1 the system reduces to the comb model where subdiffusion takes place with the transport exponent 1/2. We present an exact analytical evaluation of the transport exponent of anomalous diffusion for finite and infinite number of backbones. We show that for an arbitrarily large but finite number of backbones the transport exponent does not change. Contrary to that, for an infinite number of backbones (fractal grid comb), the transport exponent depends on the fractal dimension of the backbone structure. Thus, the grid comb model, suggested here, establishes an exact relation between a complicated fractal geometry and the transport exponent. Such a product structure of backbones times comb is an idealization of more complex comb-like fractal networks, as they may appear e.g., in certain anisotropic porous media.

CPP 5.9 Mon 11:45 BH-N 334

**On diffusivity landscapes in soft matter** — •Felix Roosen-Runge[1] and Dominique J. Bicout[1,2] — [1]Institut Laue-Langevin, Grenoble, France — [2]UMR 5525, CNRS and Université Grenoble 1, France

The concept of energy landscapes has been successfully and extensively applied for the understanding of a broad range of phenomena in complex soft matter systems, such as the glass transition and protein folding. However, many experimental accounts – e.g. single-particle tracking, scattering methods and diffusion MRI – access dynamical properties, and not the free energy landscape directly. Thus, it is important to understand and exploit the effects of diffusivity landscapes, i.e. an inhomogeneous diffusivity and viscosity. First, we discuss applicability, implications and limitations of the concept of diffusivity landscapes. Second, we provide analytical approximate solutions for the diffusion equation in dynamically heterogeneous environments. Third, the results can be connected to experiments on e.g. water diffusion in hydration shells, or tracer diffusion through membranes or porous structures.

## CPP 6: Crystallization, Nucleation and Self Assembly I (joint session CPP, DY)

Time: Monday 9:30–11:30 Location: PC 203

CPP 6.1 Mon 9:30 PC 203

**Wang-Landau type Monte Carlo study of crystallization in melts of short semi-flexible polymers** — •Timur Shakirov and Wolfgang Paul — University of Halle, Halle, Germany

Phase transitions in polymer melts have been under intensive experimental as well as theoretical investigation during the last years. Wang-Landau type Monte Carlo simulations were successfully applied to investigate of single polymer chains, but they weren't used for simulations of dense polymer systems. We present results of Wang-Landau simulations of melts of short semi-flexible polymers. The estimated density of state functions cover more than 5000 orders of magnitude and describe thermodynamical properties at the full energy range of the system. An analysis of the density of states shows that our model system undergoes a first-order phase-transition upon increasing the chain stiffness at fixed density . The investigation of chain properties demonstrates crystallization of the model system into a rotator-like phase. Because inter-molecular interactions have a purely repulsive nature, the phase transition is driven by maximization of the system entropy. Ordering perpendicular to the director is governed by the effective thickness of the chains and this part of the ordering process is similar to the transition into a hexatic phase of 2d hard-disks systems. Due to the equal size of all beads and the purely repulsive inter-chain interaction the chains remain mobile along the nematic director. So that in contrast to the real rotator-phase systems (for instance stiff n-alkane chains) our system demonstrates only a weak tendency to produce lamellar positional ordering.

CPP 6.2 Mon 9:45 PC 203

**Double-Crystalline Diblock Copolymer Nanostructures by Crystal Thickening** — •Robert Schulze, Tobias N. Büttner, and Klaus D. Jandt — Chair of Materials Science (CMS), Otto-Schott-Institute for Materials Research, Friedrich Schiller University Jena, Löbdergraben 32, 07743 Jena, Germany

Semi-crystalline diblock copolymers (DBCP) can form defined nanostructures by crystal thickening. In double-crystalline DBCP, both blocks can crystallize and, thus, be used for crystal thickening, which was not investigated, so far.

Here, the hypothesis was tested, that an increase of the lamellar period can be achieved by controlled crystal thickening of both blocks of a linear poly(ethylene)-block-poly(ethylene oxide) DBCP.

In the bulk, we found annealing induced crystal thickening for both blocks using differential scanning calorimetry. Initially crystallized bulk samples were characterized by X-ray scattering and featured a lamellar long-period that corresponded to the extended chain length of the copolymer. Similarly crystallized thin films were characterized by atomic force microscopy and the lamellar long-period was found to be one-half of the extended chain length. Annealing these thin films at elevated temperatures caused crystal thickening and an increase of the lamellar long-period.

The controlled crystal thickening of double-crystalline DBCP can be used to fabricate tailorable nanopatterns which are interesting for applications requiring surface structures with different sizes, as e.g., in photonics or the biomedical field.

**Invited Talk** CPP 6.3 Mon 10:00 PC 203

**Direct observation of prefreezing at the interface melt-solid in polymer crystallization** — Ann-Kristin Löhmann, Thomas Henze, and •Thomas Thurn-Albrecht — Institute of Physics, Martin-Luther-University Halle-Wittenberg, 06099 Halle, Germany

The microscopic ordering process that a liquid undergoes during crystallization is often initiated at an interface to a solid. This observation is classically explained by the assumption of a reduced barrier for crystal nucleation at the interface. However, an interface can also induce crystallization by prefreezing, i.e., the formation of a crystalline layer that is already stable above the bulk melting temperature. We present an atomic force microscopy (AFM)-based in situ observation of a prefreezing process at the interface of a polymeric model system and a crystalline solid, namely polyethylene on graphite. Explicitly, we show the existence of an interfacial ordered layer that forms well above the bulk melting temperature with thickness that increases on approaching melt-solid coexistence. Below the melting temperature, the ordered layer initiates crystal growth into the bulk, leading to an oriented, homogeneous semicrystalline structure.

CPP 6.4 Mon 10:30 PC 203

**Experimental test of Tammann's nuclei development approach in crystallization of macromolecules** — •Evgeny Zhuravlev[1], Jürn W.P. Schmelzer[1], and Alexander S. Abyzov[2] — [1]University of Rostock, Rostock, Germany — [2]Kharkov Institute of Physics and Technology, Kharkov, Ukraine

A first attempt to probe the size distribution of homogeneously formed nuclei in polymers was realized employing Tammann's two-stage crystal nuclei development method and fast scanning calorimetry. A transfer heating rate of 500,000 K/s prevents nuclei growth on heating in poly($\epsilon$-caprolactone). The employed temperature profile was adapted from Tammann's two-stage crystal nuclei development method implying formation of nuclei at large undercooling (low temperatures) and following their isothermal growth at higher temperatures. Fast scanning calorimetry allowed us to reach the deep supercooling of the melt at 100,000 K/s avoiding heterogeneous and homogeneous nuclei formation and growth. Then crystal nuclei were allowed to form isothermally at the temperature corresponding to the maximum of the steady-state nucleation rate for homogeneous nucleation (210 K for PCL, Tg = 209 K), where both the effect of heterogeneous nucleation and the growth rate are low. The presence of these crystal nuclei and its effect on crystallization was probed by heating the sample to higher temperatures and observation of the overall crystallization process, determining the crystallization half-time. A theoretical explanation of the observations was developed.

CPP 6.5 Mon 10:45 PC 203

**Morphological development of poly(butadiene)-block-poly(ethylene oxide) during annealing** — •Tobias N. Büttner[1], Stefan Hölzer[2], Robert Schulze[1], and Klaus D. Jandt[1] — [1]Chair of Materials Science (CMS), Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Löbdergraben 32, 07743 Jena, Germany — [2]Laboratory of Organic Chemistry and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstraße 10, 07743 Jena, Germany

Nanostructures of semi-crystalline diblock copolymers (DBCP) can be tuned by controlled crystal thickening, whereby the knowledge of the mechanisms and kinetics is relevant for possible applications.

In the present study we tested the hypothesis that the morphological development of a poly(butadiene)-block-poly(ethylene oxide) depends on the kinetics of crystal thickening during annealing and can be described by combining time- and temperature-dependent X-ray scattering (SAXS) and differential scanning calorimetry (DSC).

Depending on the annealing temperature, three effects predominated: crystal thickening, thermal fractionation and complete melting. We investigated the absolute long period growth due to crystal thickening by SAXS measurements. In addition, DSC based crystal thickness distributions were used to explain the running processes during annealing. The combination of both methods enables the precise tailoring of DBCP nanostructures without changing the degree of polymerization.

Nanostructures with defined dimensions are interesting for nanotemplating applications, e.g. the biomedical field.

CPP 6.6 Mon 11:00 PC 203

**Crystallization of binary colloidal mixtures with polymer-induced attraction** — •Nicole Schaertl[1,2], Thomas Palberg[3], and Eckhard Bartsch[1,2] — [1]Institut für Physikalische Chemie, Universität Freiburg, Deutschland — [2]Institut für Makromolekulare Chemie, Universität Freiburg, Deutschland — [3]Institut für Physik, Universität Mainz, Deutschland

Polystyrene (PS) microgel colloids serve as model system for hard spheres (HS). Binary mixtures of dispersed small (S) and large (L) PS particles with diameter ratios of S to L close to a value of $\Gamma = 0.8$ have been widely used to investigate glass formation as well as re-entrant melting introduced by short-ranged depletion attraction. Previously, we have shown that depletion attractions not only enhance particle mobility, leading to a melting of the glass, but also enforce crystallization of a colloidal eutectic which is kinetically suppressed in the corresponding HS system [1]. Here we show that a subtle change of the system parameters to slightly larger $\Gamma$ leads to a completely different enforced crystallization scenario. Using static light scattering to investigate structure and kinetics including crystal size growth and packing, we observe hexagonal superlattices instead of single-component crystals. Our findings can be rationalized by the occurrence of stable binary crystals LS2, so-called Laves phases, in agreement with computer simulations by Hynninen et al. [2].

[1] Kozina et al., Soft Matter 10, 9523 (2014) [2] Hynninen et al., J. Chem. Phys. 131, 064902 (2009)

CPP 6.7 Mon 11:15 PC 203

**Frühe Belege zur Kettenfaltung in Lamellen bei massivem HDPE** — •Heinz Preuss — 31785 Hameln

Mit dem Oberflächenabriss von aus der Schmelze bei langsamer Abkühlung erstaarrten massiven Proben aus Niederdruckpolyethlen (HD-PE) gelang die mechanische Trennung der Lamellen längs ihrer Grenzflächen (H.H.W.Preuß, physica status solidi Vol. 3, 1963 S. K209 ff.). Dies belegt sowohl, dass die in elektronenmikroskopischen Oberflächenbildern sichtbaren Terrassenstufen tatsächlich die Ränder von Lamellen sind, die sich als relativ selbständige Struktureinheiten in das Probeninnere fortsetzen, als auch die schwächere Bindung der Lamellen aneinander. Zugleich erfährt das Modell der Kettenfaltung (z. B. A. Keller, Kolloid * Zeitschrift, 165 (1959), s. 15) eine Bestätigung. Mit dessen Hilfe lässt sich erklären, dass die Molekülketten, welche senkrecht zu den Lamellengrenzflächen orientiert sind, sich in den Lamellen kristallografisch geordnet in den Lamellen unterbringen lassen, obwohl deren Dicke D (8 bis 15 nm) deutlich kleiner ist als die Kettenlänge L.

## CPP 7: Organic Electronics and Photovoltaics

Time: Monday 9:30–13:00 Location: H 2032

CPP 7.1 Mon 9:30 H 2032

**Metal-organic interfaces: from molecular self-assembly to electronic transport through ultrathin functional monolayers** — •Florian von Wrochem — Sony Deutschland GmbH, Stuttgart

The continuous development of organic electronic devices, combined with the advances in spectroscopy and electrical characterization, dramatically extended our understanding of the physical and chemical processes occurring at metal/organic interfaces. Here, an overview of experimental and theoretical efforts aiming towards the selective modification of interfaces is given. Various anchor groups designed to connect organic materials to metal electrodes are presented (e.g. thiolates, dithiocarbamates, mercuryls and stannyls) and their potential for optimizing the charge injection as well as the morphological, chemical, and electronic nature at the contact is illustrated. On this basis, functional molecular building blocks are grafted to the surface by self-assembly, providing rectification, switching, or chemical selectivity. Once the key parameters for interface formation and fabrication are under control, a huge number of potential applications emerge, ranging from optoelectronics to organic printed circuits. As one example, electrostatic dipole layers for tuning the injection barrier between metals and organic semiconductors are presented, which may find applications in organic light emitting diodes, field effect transistors, and solar cells. When further reducing device dimensions towards the nanoscale, organic monolayers might foster the development of molecular electronics, as illustrated here by highly robust metal-molecule-metal junctions based on FeII-terpyridine molecular wires or by optically switchable protein layers.

CPP 7.2 Mon 9:45 H 2032

**Grain boundaries in $CuInSe_2$ and $CuGaSe_2$ solar cell materials: New insights from hybrid functional calculations** — Hossein Mirhosseini, •Janos Kiss, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany.

Polycrystalline thin-film solar cells based on $CuIn_{1-x}Ga_xSe$ (CIGSe) are an economically viable alternative to the Si based technology. During the deposition of the polycrystalline light absorber layer grain boundaries (GBs) are formed in the CIGSe material, and the effect of these GBs upon the structural and electronic properties of the thin-film solar cells are not yet fully understood. Different atomic structures of the GBs in CIGSe have been reported experimentally. The outcomes of the theretical calculations, however, are diverse and sometimes inconsistent due to the limitation of the functionals, which fail to properly describe the band gap of thin film solar cell materials. Employing a state of the art method using the HSE hybrid functional, which is known to predict the atomic and electronic structure of solar cell materials rather well, we have looked at the behavior and properties of GBs in $CuInSe_2$ and $CuGaSe_2$. In the framework of our investigation, we have studied the atomic relaxation and electronic structure of various GBs and also considered the effect of the impurity segregation close to the GBs.

CPP 7.3 Mon 10:00 H 2032

**Relationship between the chemical structure of low band gap polymers and self-organization properties** — •Milutin Ivanovic[1], Umut Aygül[1], Ulf Dettinger[1], Aurelien Tournebize[1], David Batchelor[2], Stefan Mangold[2], Heiko Peisert[1], and Thomas Chassé[1] — [1]) University of Tuebingen, Institute of Physical and Theoretical Chemistry, 72076 Tuebingen, Germany — [2]Karlsruhe Institute of Technology (KIT), ANKA Synchrotron Radiation Facility, 76344 Eggenstein-Leopoldshafen, Germany

A possible approach to improve the efficiency of donor-acceptor based bulk heterojunction (BHJ) of OPV cells is the use of low band gap (LBG) polymers as donor materials. Basic electronic processes in OPV cells are however strongly influenced by the morphology and the ability for self-organization of the polymers in the thin-films. We utilize NEXAFS spectroscopy to study the molecular orientation of novel LBG polymers (PCPDTTBBTT, PCPDTTBTT and PCPDTzTBTT) for OPVs in thin films. The influence of post-processing annealing as well as of blending with Phenyl-C61-butyric acid methyl ester (PCBM) on the orientation is investigated. The studied LBG polymers are characterized by a variation of (hexyl-) thiophene groups compared to related LBG polymers recently studied.[1,2]. Acknowledgments: This research is funded by the European Union Seventh Framework Programme (FP7/2011 under grant agreement ESTABLIS n° 290022). References: 1.*Aygül, U. et al. J. Phys. Chem. C 2012, 116, 4870-4874. 2.*Aygül, U. et al. Sol. Energ. Mat. Sol. Cells 2014, 128, 119-125.

CPP 7.4 Mon 10:15 H 2032

**Organic ambipolar field-effect transistors: *In situ* electrical investigation of MnPC-OFETs** — •Franziska Lüttich, Ovidiu D. Gordan, and Dietrich R. T. Zahn — Semiconductor Physics, Technische Universität Chemnitz, Chemnitz, Germany

On the way to low-cost and flexible applications organic semiconducting materials are promising. Devices like organic light-emitting diodes, organic solar cells, and organic field-effect transistors (OFETs) can be produced *e.g.* on flexible and elastic substrates and with chemical variation of side groups or substitution of metal centers their properties like optical absorption and charge carrier mobilities can be influenced.

Here we present a temperature dependent study on Manganese Phthalocyanine (MnPc)-OFETs, which reveal an ambipolar behaviour. In order to investigate the electrical properties of MnPc we used OFET "'end-of-line"' substrates from Fraunhofer IPMS with a 100 nm thick thermal silicon dioxide layer as dielectric. The investigated bottom-contact OFETs were fabricated under high vacuum conditions ($p < 4 \cdot 10^{-7}$ mbar) by evaporating MnPc on top of the pre-structured substrates. The electrical DC characteristics were measured *in situ* as a function of temperature. This procedure enables us to determine the activation energies for the hole and electron transport. The influence of ambient atmosphere was also investigated and revealed strong impact on the electrical performance. The topography was determined using an Atomic Force Microscope (AFM).

CPP 7.5 Mon 10:30 H 2032

**Photoelectron spectroscopy studies on efficient air-stable molecular n-dopants** — •Martin Schwarze[1], Max L. Tietze[1], Paul Pahner[1], Ben Naab[2], Zhenan Bao[2], Björn Lüssem[1], Daniel Kasemann[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Department 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 such as organic light emitting diodes or organic solar cells. A defined doping concentration allows for the control of the Fermi-level position as well as the adjustment of the conductivity of transport layers. In comparison to molecular p-doping of organic semiconductors, n-doping creates 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: air stable cationic DMBI dopants, halogen-free DMBI dimers, and the established but air sensitive Cr2(hpp)4. Fermi-level shift and conductivity of co-evaporated Bis-HFl-NTCDI layers at different doping concentrations as well as stability during air exposure are investigated by UPS and electrical measurements.

CPP 7.6 Mon 10:45 H 2032

**Mode-selective vibrational manipulation of charge transport in $\pi$-conjugated molecular materials** — •Robert Lovrincic[1,2], Artem A. Bakulin[3,4], Yu Xi[1], Oleg Selig[3], Huib J. Bakker[3], Yves L. A. Rezus[3], Pabitra K. Nayak[1], Alexandr Fonari[5], Veaceslav Coropceanu[5], Jean-Luc Bredas[5,6], and David Cahen[1] — [1]Department of Materials & Interfaces, Weizmann Institute of Science, Israel — [2]IHF, TU Braunschweig & Innovationlab, Germany — [3]FOM Institute AMOLF, The Netherlands — [4]Cavendish Laboratory, University of Cambridge, UK — [5]School of Chemistry and Biochemistry , Georgia Institute of Technology, USA — [6]Solar & Photovoltaics Center, King Abdullah University, Saudi Arabia

The soft character of organic materials leads to strong coupling between molecular nuclear and electronic dynamics. This coupling opens the way to control charge transport in organic electronic devices by directing molecular vibrational motions. However, despite encouraging theoretical predictions, experimental realization of such control has remained elusive. Here we demonstrate experimentally that photoconductivity in a model organic optoelectronic device can be controlled by the selective excitation of molecular vibrations. Using an ultrafast infrared laser source to create a coherent superposition of vibrational motions in a pentacene/C60 photoresistor, we observe that excitation of certain modes in the $1500 - 1700\,\mathrm{cm}^{-1}$ region leads to photocurrent enhancement. The effect depends on the nature of the vibration and its mode-specific character can be well described by the vibrational modulation of intermolecular electronic couplings.

CPP 7.7 Mon 11:00 H 2032

**Investigation of charge transfer in organic semiconductors using infrared spectroscopy** — •Tobias Glaser[1,2], Sebastian Beck[1,2], and Annemarie Pucci[1,2,3] — [1]Universität Heidelberg, Kirchhoff-Institut für Physik — [2]InnovationLab GmbH, 69115 Heidelberg — [3]Universität Heidelberg, Centre for Advanced Materials

Charge transfer in organic semiconductors is used in various ways to increase the performance of organic electronic devices. For example electrochemical doping is used to increase the conductivity in charge transport layers. Additionally, charge injection layers are used to decrease injection barriers between electrodes and organic transport layers. In both cases molecular charge transfer plays an important role, but the basic mechanisms are still subject of heated debate. Due to strong relaxation effects upon molecular charging, infrared (IR) spectroscopy is very well suited to investigate charge transfer in organic semiconductors. Neutral and charged molecules can be distinguished by their different specific vibrational features in spectra of doped layers as well as for interfaces. In this study we investigated charge transfer in thin layers of commonly known transport materials such as 4,4*-bis(N-carbazolyl)-1,1*-biphenyl (CBP) doped with inorganic and organic dopants such as MoO3 or F4TCNQ and at interfaces of organic semiconductors. By quantitative analysis of the experimental spectra the doping efficiency and the degree of charge transfer can be determined for the doped layers. Whereas, for interfacial charge transfer, the formation of a space charge region can be mapped. Financial support by BMBF (project MESOMERIE) is gratefully acknowledged.

CPP 7.8 Mon 11:15 H 2032

**Structure and Photovoltaic Performance of Chiral Anilino Squaraines** — •Manuela Schiek[1], Matthias Schulz[2], Stefanie Brück[1], Martin Silies[3], Heiko Kollmann[3], Christoph Lienau[3], Arne Lützen[2], and Jürgen Parisi[1] — [1]Energy and Semiconductor Research Laboratory, University of Oldenburg, Germany — [2]Kekule-Institute for Organic Chemistry and Biochemistry, University of Bonn, Germany — [3]Ultrafast Nano-Optics, University of Oldenburg, Germany

Small molecular semiconductors such as squaraines are advantageous compared to polymeric materials because they allow a more direct control of the structure on the molecular level and consequently solid state properties. Especially the implementation of chiral side chains introduces new functionalities such as circular dichroism. Different 1,3-bis(N,N-substituted-2,6-dihydroxy-anilino)squaraines with varying terminal N-substitution, in some cases including a stereogenic center, are investigated as single crystals, in thin films and blended with a fullerene acceptor as active layer in bulk heterojunction organic solar cells.

CPP 7.9 Mon 11:30 H 2032

**Charge separation and C$_{60}$ crystallinity in bulk heterojunction solar cells: the decisive role of device architecture** — •Felix Schell[1,2], Michael Scherer[1,3], Diana Nanova[1,2,3], Anne Katrin Kast[2,4], Wolfgang Kowalsky[1,2,3], Rasmus R. Schröder[1,4,5], and Robert Lovrincic[1,3] — [1]InnovationLab GmbH, Heidelberg — [2]Kirchhoff-Institute for Physics, Heidelberg University — [3]Institute for High-Frequency Technology, TU Braunschweig — [4]CellNetworks, BioQuant, Heidelberg University — [5]Center for Advanced Materials, Heidelberg University

The crucial influence of C$_{60}$ crystallinity on the charge separation in organic solar cells (OSC) has been realized very recently. Here, we show the importance of the device architecture on C$_{60}$ crystallisation in the bulk-heterojunction (BHJ). Active layer morphology of small molecule BHJ OSC and its influence on device performance are studied by means of energy-filtered transmission electron microscopy (EFTEM) and electrical characterization. The influence of substrate temperature during deposition and of pure sublayers is assessed. BHJs fabricated at room temperature are found to be finely mixed and amorphous, whereas the corresponding films deposited onto heated substrates show pronounced phase separation. Despite these clear morphological changes, substrate heating does not increase efficiency of OSCs in a non-inverted device architecture. Improvements found in literature for inverted cells can be attributed to stronger acceptor crystallization, present, if deposited onto a pure C$_{60}$ layer but not with an F$_4$ZnPc substrate, leading to more efficient exciton dissociation.

CPP 7.10 Mon 11:45 H 2032

**Influence of DMSO-treatment on morphology, composition and performance of PEDOT:PSS layers in organic photovoltaic cells** — Sidhant Bom, •Torsten Balster, Marlis Ortel, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

PEDOT:PSS layers in organic solar cells are used as hole transport (HTL) and electron blocking layers. Therefore the morphology and composition of the layer and the interface have a great influence on the performance of organic photovoltaic devices.

Additional post-deposition treatment of the PEDOT:PSS layers (HTL) in P3HT/PCBM solar cells were studied in this work. For this purpose, pristine PEDOT:PSS layers were spin coated with dimethyl sulfoxide (DMSO) after annealing. Pristine and treated layers were characterized by means of electrical characterization, atomic force microscopy (AFM) and x-ray photoelectron spectroscopy (XPS).

The additional post-deposition DMSO treatment induces an increase in power conversion efficiency by more than 50%. In addition, the open circuit voltage and the short-circuit current were enhanced, whereas the fill factor remained constant. This behavior is explained by modification of the PEDOT:PSS-semiconductor interface. On the one hand smoothening of the interface by reduction of large PSS particles visible in AFM occurs. On the other hand XPS data show a reduction of PSS-sulphur species. Less PSS at the interface should improve the charge carrier injection properties, as observed experimentally.

CPP 7.11 Mon 12:00 H 2032

**Charge transfer, optical and transport properties in pure organic heterostructures** — •Liebing Simon, Hahn Torsten, and Kortus Jens — Institute of Theoretical Physics, TU Bergakademie Freiberg, Leipziger Strasse 23, 09599 Freiberg

We will present theoretical investigation on pure charge transfer materials within the density functional theory framework (DFT). Starting from the recently fabricated picene-F$_4$TCNQ [1] we explore the electronic and optical properties of novel representatives of this new class of materials. These representatives are formed of polycyclic hydrocarbons and TCNQ derivatives and we compare our results with experimental spectroscopic data.

The picene-F$_4$TCNQ system shown pronounced diode transistor behavior [2]. By means of DFT/NEGF (non equilibrium green function formalism) [3,4] we obtain the IV-characteristics of selected model devices for these systems. The formation of hybrid orbitals together with intrinsic charge transfer seems to be the origin of the novel electronic and transport properties [5].

[1] Mahns, B. et. al. Crystal Growth & Design (2014). [2] Hahn T., Liebing S., and Kortus J., Nanoscale 6, 14508 (2014). [3] Pederson, M. et. al. Phys. Status Solidi b 217, 197. (2000) [4] Enkovaara, J. et al. Journal of Physics: Condensed Matter 22, 253202 (2010). [5] Lindner S. et. al. Phys. Rev. Lett. 109, 027601 (2012).

CPP 7.12 Mon 12:15 H 2032

**Single molecule circuits with N-heterocyclic carbene linkers** — •Hector Vazquez — Inst. of Physics, Academy of Sciences of the Czech Rep., CZ

In single molecule circuits, where an electrical current flows through a molecule, conducting molecules often have terminal linker groups which bind to the metallic electrodes [1]. These chemical link groups strongly influence the conducting properties, often acting as bottlenecks for electron transmission and result in low-transmission resonances localized at the interface. Therefore, identifying adequate chemical linker groups is essential for achieving ideal mechanical and conducting properties in molecular circuits.

Recently, SAMs of N-heterocyclic carbenes on gold were shown to have very high thermal and oxidative stability [2], making N-heterocyclic carbenes potentially very useful linkers for single molecule transport. In this talk, I will present results from first-principles simulations based on DFT-NEGF for the electronic and conducting properties of carbene-terminated molecules. I will show results for the adsorption properties of N-heterocyclic carbenes on gold. I will also present transmission calculations of carbene-terminated molecules and discuss these results in the context of other metal-molecule links with Au-C bonds [3].

[1] F. Schwarz and E. Loertscher, J. Phys. Condens. Matter 26 474201 (2014).

[2] C.M. Crudden et al., Nature Chemistry 6 409 (2014).

[3] W. Chen et al., J. Am. Chem. Soc. 133 17160 (2011).

CPP 7.13 Mon 12:30 H 2032

**Charge and spin transfer materials for molecular electronic and spintronic applications** — •Torsten Hahn, Simon Liebing, and Jens Kortus — TU Freiberg, Institut für Theoretische Physik, Leipziger Str. 23, 09599 Freiberg

The combination of different functionalized metal phthalocyanines was found to lead to novel charge- and spin transfer compounds [1,2]. The recently synthesized picene / F4TCNQ charge transfer salt [3] also shows promising physical properties and the theoretical modeling predicts the material to act as a molecular diode with high rectification ratio [4]. Based on density-functional theory calculations we show that in case of the metal phthalocyanines as well as for the picene / F4TCNQ system hybrid states formed by the donor / acceptor system are playing the key role to determine the spectroscopic and quantum transport properties. We further conclude that the tuning of quantum transport properties through hybrid states is a general concept which opens a new route towards functional materials for molecular electronics.

[1] R. Friedrich et al., Phys. Rev. B 87, 115423 (2013). [2] R. Friedrich, B. Kersting, and J. Kortus, Phys. Rev. B 88, 155327 (2013). [3] Mahns, B. et. al., Cryst. Growth and Design 14, 1338-1346 (2014). [4] T. Hahn, S. Liebing, and J. Kortus, Nanoscale 6, 14508 (2014).

CPP 7.14 Mon 12:45 H 2032

**Device-like calcium corrosion test for ultra-barrier materials** — •Frederik Nehm[1], Hannes Klumbies[1], John Fahlteich[2], Felix Dollinger[1], Karl Leo[1], and Lars Müller-Meskamp[1] — [1]Institut für Angewandte Photophysik, TU Dresden, Dresden, Deutschland — [2]Fraunhofer FEP, Dresden, Deutschland

The continuous progress of organic electronics demands for flexible moisture barriers with water vapor transmission rates (WVTRs) below $10^{-4}\,\frac{g(H_2O)}{m^2 d}$ and quick, reliable measurement techniques for such WVTRs. The electrical calcium corrosion test is an extremely sensitive technique used widely in research groups. However, setups differ strongly as do their accuracy and background rates. We report on common issues and show how we manage them in our setup. Barrier corrosion because of direct water condensation on its surface is prevented by a glued-on PET film and Ca-induced stress is mitigated by organic decoupling layers. We demonstrate the effectiveness of our approach with studies on sputtered Zinc-Tin-Oxide and atomic layer deposited (ALD) alumina moisture barriers in different aging climates. Single barriers show a linear WVTR increase with rising absolute humidity at given temperature. Below $40^\circ C$, this is even valid independent of temperature. A divergence at higher temperatures probably originates from the actual barrier layer, since this effect cannot be observed for the pure substrate. Also, nanolaminates using ALD alumina, titania and alkoxide, and multilayer barriers with polymer interlayers with WVTRs down to at least $2 \cdot 10^{-5}\,\frac{g(H_2O)}{m^2 d}$ in $38^\circ C$, 90% relative humidity environments are investigated.

# CPP 8: Colloids and Complex Liquids II (joint session CPP, BP, DY)

Time: Monday 15:00–18:45 Location: C 130

CPP 8.1 Mon 15:00 C 130

**TIRM at liquid/liquid interfaces** — •Kilian Dietrich — University of Stuttgart, Germany

Total Internal Reflection Microscopy (TIRM) is a well-established method for the direct measurement of interaction potentials between a spherical colloidal particle and a solid wall. It is based on the tracking of the particle's vertical motion from which interaction forces with the interface can be inferred with a resolution down to 10fN. In contrast to previous measurements, which were performed at solid/liquid interfaces, here we demonstrate that TIRM can be applied also to liquid/liquid interfaces. These are of special interest not only due to their frequent appearance but they also exhibit an exceptional smoothness. In our study, we present a novel inverted TIRM apparatus which is capable to measure the motion of a colloidal probe particle in water close to an oil-water interface. First measurements indicate the counterplay of electrostatic interactions and van-der-Waals forces for interfaces treated with different ionic and non-ionic surfactants. In each case surface charge densities of particle and interface could be determined. The detailed knowledge of interactions can provide valuable information for the stability of emulsions and dispersions.

CPP 8.2 Mon 15:15 C 130

**Short Ranged Repulsive Energy in Oscillatory Structural Forces** — •Sebastian Schön and Regine von Klitzing — Technische Universität Berlin Strasse des 17. Juni 124 D-10623 Berlin

Oscillatory structural forces are a genuine feature observed for simple and complex fluids in the vicinity of smooth wall. The origin of these forces is related to the characteristic quality of molecules or nanoparticles to form well-ordered layers in the vicinity of a confining wall. These forces can be described by the following function as proposed by Israelachvilli: f(x)=-A*e^(-x/$\xi$)*cos(2$\pi$(x-$\Delta$x)/$\lambda$), with f the force as a function of x, the separation. The Amplitude A describes the strength of the particle interaction, the decay length $\xi$ is a measure of how fast the order decays and the wavelength $\lambda$ is directly related to the inter-particle distance. Structural oscillation forces are long ranged compared to the common DLVO forces and can be used in a variety of applications e.g. oil removal or separation of bidisperse particle suspensions For both it is important to know the strength of the oscillatory forces at very small separations. An additional repulsive term is introduced to describe deviations observed between experimental data and the common fit function, this allows accurate fitting of experimental data down to very small separations and removes systematic deviations in A, $\lambda$ and $\xi$ depending on the starting point of the fit. The short ranged repulsive energy described by the new term is investigated at different particle concentrations, measurement speed and under the addition of NaOH, HCl and NaCl at different concentrations.

CPP 8.3 Mon 15:30 C 130

**Complex nanoparticle arrangements via wrinkle-assisted self-assembly** — •Christoph Hanske, Moritz Tebbe, Christian Kuttner, Munish Chanana, Tobias König, and Andreas Fery — Physical Chemistry II, University of Bayreuth, 95447, Germany

Template-assisted assembly enables the arrangement of colloidal particles into well-defined structures that often demonstrate special optical, biological, or catalytic functionality due to the hierarchical internal organization. A major bottleneck so far is the limited scalability of lithographic template fabrication. As an alternative strategy, we utilize wrinkled elastomer substrates exhibiting periodicities on the micron or submicron scale. The topographic features of such templates allow the arrangement of hydrophilic nanoparticles into regular, close-packed chains, which can further be transferred site-selectively onto flat substrates by wetting controlled printing. This versatile method is applicable for polymeric, inorganic and metallic particles with spherical as well as anisotropic shapes. We discuss the influence of interfacial properties originating from the employed particle and substrate coatings and demonstrate the formation of complex structures on chemically patterned substrates.[1] Further, the realization of macroscopic, gold nanoparticle assemblies is shown.[2, 3] Due to small interparticle distances of few nanometers, strong plasmonic coupling is achieved, which grants access to surfaces with tailored optical properties.

[1] C. Hanske et al., Langmuir, 2012, 28, 16745-16750. [2] C. Hanske et al., Nano Letters, 2014, DOI:10.1021/nl502776s. [3] M. Tebbe et al., submitted.

CPP 8.4 Mon 15:45 C 130

**Linking intermolecular interactions, microstructure, and macroscopic rheology in protein suspensions** — •Alessio Zaccone[1], Miriam Siebenbürger[2], Henning Winter[3], Frank Schreiber[4], and Matthias Ballauff[2] — [1]Physics-Department, Technische Universität München — [2]Helmholtz-Zentrum Berlin für Materialien und Energie — [3]University of Massachusetts Amherst — [4]Applied Physics, University of Tübingen

We propose a microscopic framework based on nonequilibrium statistical mechanics to connect the microscopic level of colloidal biopolymer self-assembly with the macroscopic rheology of protein gelation. The method is based on the master kinetic equations for the time evolution of the self-assembled cluster size distribution, from which the relaxation time spectrum during the gelation process can be extracted. The relaxation spectrum is a simple stretched-exponential, with a stretching exponent related to the mass fractal dimension of the self-assembling clusters. In the case of thermoreversible gelation, for weak interparticle attractions, the attraction energy is finite and plays the role of the control parameter driving a nonequilibrium phase transition into a nonequilibrium steady-state ( the gel). Our theory is in good agreement with experimental data of different systems published by other authors, for which no theory was available. Further, it allows us to interpret new experimental data on the gelation of BSA which provides a benchmark system to connect the level of coarse-grained protein interactions with the macroscopic oscillatory rheology of the protein suspension.

CPP 8.5 Mon 16:00 C 130

**Molecular versus macroscopic perspective on the phase separation mechanisms of thermo-responsive solutions** — •Martine Philipp[1], Ralitsa Aleksandrova[2], Ulrich Müller[2], Jan K. Krüger[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, Garching, Germany — [2]Université du Luxembourg, LPM, Luxembourg, Luxembourg

The phase separation of thermo-responsive solutions is known to strongly affect the volume expansion behaviour and the elastic properties, being directly coupled to the macroscopic order parameter [1-3]. On the molecular scale, massive changes in H-bond and hydrophobic interactions, and in structure govern the demixing process. However, the relationship between the molecular and macroscopic order parameters is poorly understood for such complex segregating solutions. We contribute to the clarification of this problem by first following the diffusion behaviour of the hydration water across the phase transition of model aqueous poly(N-isopropylacrylamide) solutions using quasi-elastic neutron scattering [2]. By probing the molecular bond polarisabilities, we adopt an alternative, highly revealing perspective on the changes in molecular interactions and in structure happening within dilute to concentrated phase-separating solutions [1, 3]. [1] M. Philipp, et al., Soft Matter 10, 7297-7305 (2014), [2] M. Philipp, et al., J. Phys. Chem. B 118, 4253-4260 (2014), [3] R. Aleksandrova, et al., Langmuir 30, 11792-11801 (2014)

CPP 8.6 Mon 16:15 C 130

**Cononsolvency in P(S-*b*-NIPAM) diblock copolymers - a time-resolved SANS study of the aggregation process** — Konstantinos Kyriakos[1], Martine Philipp[1], Joseph Adelsberger[1], Sebastian Jaksch[1], Anatoly V. Berezkin[1], Dersy M. Lugo[2], Walter Richtering[2], Isabelle Grillo[3], Anna Miasnikova[4], André Laschewsky[4], Peter Müller-Buschbaum[1], and •Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching — [2]RWTH Aachen University, Institut für Physikalische Chemie — [3]Institut Laue-Langevin, Grenoble, France — [4]Universität Potsdam, Institut für Chemie, Potsdam-Golm

In mixtures of water and methanol, the thermoresponsive poly(N-isopropylacrylamide) (PNIPAM) exhibits the cononsolvency effect, i.e. an enhanced tendency for phase separation at certain solvent compositions. We investigate the effect of adding methanol to (i) micellar solutions of polystyrene-*b*-poly(N-isopropylacrylamide) (PS-*b*-PNIPAM) diblock copolymers and (ii) PNIPAM homopolymers in $D_2O$ using a stopped-flow instrument. The structural changes on mesoscopic length scales were followed by time-resolved small-angle neutron scattering (TR-SANS) with a time resolution of 0.1 s. In both systems, the pathway of the aggregation depends on the content of deuterated methanol; however, it is fundamentally different for homopolymer and diblock copolymer solutions. We propose a logarithmic coalescence model based on an energy barrier which is proportional to the aggregate radius.

1. Kyriakos et al., *Macromolecules* **47**, 6867 (2014)

CPP 8.7 Mon 16:30 C 130

**Cation-activated attractive patches to control protein interactions** — •Felix Roosen-Runge[1], Fajun Zhang[2], Frank Schreiber[2], and Roland Roth[3] — [1]Institut Laue-Langevin, Grenoble, France — [2]Institut für Angewandte Physik, Universität Tübingen — [3]Institut für Theoretische Physik, Universität Tübingen

We present evidence for an explicit ion-activated mechanism to cause a patchy attraction between proteins [1]. Experimentally, ion bridges of multivalent cations between protein molecules have been observed in protein crystals [2]. Modeling this mechanism via particles with ion-activated attractive patches, a broad variety of experimental results for protein solutions with multivalent cation is explained and understood very naturally, including charge reversal, reentrant condensation, metastable liquid-liquid phase separation, cluster formation and different pathways of crystallization [1,3]. The good agreement between theory and experiments indicates that protein-cation solutions represent a natural model system for patchy particles. The mechanism of ion-activated patches can be embedded seamlessly into theory and simulations of charged soft matter, and promises rational design of phase behavior and crystallization pathways in protein solutions based on the statistical physics of patchy particles.

[1] F. Roosen-Runge, F. Zhang et al. *Sci. Rep.* 4 (2014) 7016
[2] F. Zhang, A. Sauter et al. *J. Appl. Cryst.* 44 (2011) 755
[3] F. Zhang, R. Roth et al. *Soft Matter* 8 (2012) 1313

CPP 8.8 Mon 16:45 C 130

**Buckling of paramagnetic chains in soft gel** — •Shilin Huang and Günter K. Auernhammer — Max Planck Institute for Polymer Research, Mainz, Germany

We study the magneto-elastic coupling behavior of paramagnetic chains in a soft polymer gel. To this end, the laser scanning confocal microscope is used to observe the morphology of the paramagnetic chains as well as the deformation field in the polymer gel. The paramagnetic chains in a soft polymer gel show rich morphologies under an oblique magnetic field. Depending on the chain length, the chains rotate, bend and buckle. In a perpendicular magnetic field, longer chains form wavy structure with higher number of buckles. A higher magnetic field strength and a lower modulus of gel matrix lead to higher amplitude of the buckling. The deformation field around a deformed magnetic chain confirms that the polymer network is strongly coupled with the paramagnetic chain. A theoretical model is developed to describe the buckling of the chain.

**15 min. break**

CPP 8.9 Mon 17:15 C 130

**Environmentally compatible microemulsion at solid surfaces: Wetting behavior and extraction properties** — •Salomé Vargas Ruiz[1], Christoph Schulreich[2], Ramasia Sreich[2], Martin Jung[3], Regine von Klizing[1], Thomas Hellweg[2], and Stefan Wellert[1] — [1]Stranski Laboratory, TU Berlin, Str. d. 17 juni 124, 10623 Berlin, Germany — [2]Physical Chemistry III, University Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany. — [3]Armed Forces Scientific Institute for NBC Protection, Humboldtstraße 1, 29633 Munster, Germany.

Microemulsions based on sugar surfactants and food grade oil are potential decontamination media for the remediation of sorptive surfaces exposed to highly toxic compounds (e.g nerves agents, pesticides). The main advantage of microemulsions relies on their capability to degradate the solubilized toxic compound by means of active ingredients hosted in the water phase. Although microemulsions have good performance on the detoxification process, the overall efficiency of the decontamination process is also determined by their ability to wet the treated surfaces and to extract the contaminants. In this study, we examined firstly the wettability and penetration properties of microemulsion formulated with sugar surfactant SL55 and methyl oleate oil, and secondly we evaluated their ability to extract lipophilic contaminants via spectroscopic and chromatographic techniques. Here, the formulated microemulsions can wet and penetrate hydrophobic and hydrophilic sorptive surfaces and their extraction properties are greatly influenced by their structure and oil content.

CPP 8.10 Mon 17:30 C 130

**Supramolecular structure of pure and mixed monohydroxy alcohols** — •Thomas Büning[1], Christian Sternemann[1], Sebastian Peter Bierwirth[1], Catalin Gainaru[1], Jennifer Bolle[1], Michael Paulus[1], Christoph J. Sahle[2], Roland Böhmer[1], and Metin Tolan[1] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, D-44221 Dortmund, Germany — [2]European Synchrotron Radiation Facility (ESRF), F-38000 Grenoble, France

Hydrogen bonds are essential for the structure and dynamics of alcohols, aqueous solutions, and water. Due to their low tendency of crystallization and large variability in molecular configuration, monohydroxy alcohols (MAs) are often studied as model systems for hydrogen-bonded fluids in general [1]. MAs are supposed to form supramolecular structures such as chains and rings via hydrogen bonding in the liquid phase. Based on their small dielectric absorption, ringlike arrangements were suggested for neat MAs with a sterically hindered polar hydroxyl group [1], e.g., for 4-methyl-3-heptanol and 2-hexyl-1-decanol. Mixtures of these MAs show a significantly enhanced dielectric absorption which hints at a change of supramolecular topology [2]. We present combined X-ray diffraction and X-ray Raman measurements of MA mixtures. Here, the first X-ray diffraction peak and the shape of the oxygen K-edge, respectively, are sensitive to the local arrangement of MAs. The results are interpreted with respect to a transformation from ringlike to chainlike structures upon mixing. [1] R. Böhmer et al. Phys. Reports 545 125-195 (2014) and references therein; [2] S. P. Bierwirth, et al. Phys. Rev. E 90, 052807 (2014).

CPP 8.11 Mon 17:45 C 130

**The role of the cation and polarization on lithium ion coordination in ionic liquids** — •Volker Lesch[1], Zhe Li[2], Dmitry Bedrov[2], and Andreas Heuer[1] — [1]Westfälische Wilhelms-Universität Münster — [2]University of Utah

MD-simulations are a powerful tool to investigate microscopic processes in complex systems as ionic liquids. The interactions between the cation and the anion are only weak but in the case of adding lithium to an ionic liquid the anions strongly interact with this small lithium ion. The role of the cation on this interaction was never investigated.

Here, we compare the cations 1-ethyl-3-methylimidazolium with N-metyhl-N-propylpyrrolidium and as counterion bis-(trifluoromethanesulfonyl)-imide was used. Both cations differ in size and viscosity but on the microscopic scale only a comparison for pure ionic liquids is published. We performed MD-simulations for the two ionic liquids doped with lithium salts at different temperatures and different oxygen polarizations. The change of the TFSI oxygen polarization was necessary due to new DFT calculations that predicts the $Li^+$ - $Ntf_2$ binding energy more accurate. We observed a dramatic influence of the polarization on structural properties while the dynamics are only slightly affected. The comparison of the cations shows only small differences for the lithium ion coordination.

CPP 8.12 Mon 18:00 C 130

**A systematic study of the influence of trivalent metal ions on phase behaviour in protein solutions** — •Olga Matsarskaia[1], Michal Braun[1], Andrea Sauter[1], Marcell Wolf[1], Roland Roth[2], Fajun Zhang[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]Institut für Theoretische Physik, Universität Tübingen

Thermodynamic phenomena such as reentrant condensation (RC) and liquid-liquid phase separation (LLPS) are involved in various protein-related processes, e.g. protein condensation diseases and protein crystallisation. We could show that these transitions are inducible in protein solutions using various trivalent cations [1], [2]. In this work, the influence of cation size on such phase behaviour in bovine serum albumin (BSA) was studied systematically in the presence of salts with increasing cation sizes ($YbCl_3$, $YCl_3$, $GdCl_3$, $CeCl_3$ and $LaCl_3$). The results reveal that charge inversion, the prerequisite of RC and LLPS in these systems, is found independent of cation size. Interestingly, however, salt concentration ranges in which macroscopic LLPS is observed decrease with increasing cations: while $Yb^{3+}$ leads to the largest LLPS area, $Ce^{3+}$ features the smallest one. $La^{3+}$, the largest cation studied, induces RC, but does not lead to LLPS at all. The findings thus indicate that the size of cations present in the environment of a protein influences the strength of protein-cation interactions and therefore plays an important role in phase transitions of the protein.

[1] Zhang et al (2008). Phys. Rev. Lett., 101(14), 148101; [2] Zhang et al (2012). Soft Matter, 8, 1313-1316.

CPP 8.13 Mon 18:15 C 130

**New relaxation process for water in electric fields** — •Zoran Miličević[1], David M. Smith[2,3], and Ana-Sunčana Smith[1,3] — [1]Institut für Theoretische Physik and Cluster of Excellence: Engineering of Advanced Materials, FAU Erlangen-Nürnberg, Erlangen, Germany — [2]Computer Chemie Centrum, FAU Erlangen-Nürnberg, Erlangen, Germany — [3]Ruđer Bošković Institute, Zagreb, Croatia

Despite a heavily increasing number of electrochemical applications, theoretical and experimental studies of solvent shear properties in the presence of electric fields are almost non-existent. Here we study the shear viscosity of water by performing extensive MD simulations using the GROMACS software package as a function of the electric field strength which breaks the otherwise isotropic nature of the solvent. The shear viscosity is related to the autocorrelation function (ACF) of the off-diagonal elements of the pressure tensor by the Green-Kubo relation. The value of the shear viscosity is determined from the plateau value of the time integral of the ACF or, alternatively, by exploiting the Kohlrausch fit curve of the ACF using a uniform 2-step (fast plus slow) relaxation function. Apart from the fact that the two approaches show an excellent agreement, we find that the field decreases the component of the shear viscosity perpendicular to itself and increases the components which are parallel. Importantly, the field induces an additional slow relaxation process (decoupled from the fast relaxation) only in the parallel direction, increasing by about tenfold the total relaxation time with respect to the perpendicular direction. Furthermore, the overall water shear viscosity increases slightly with the field strength.

CPP 8.14 Mon 18:30 C 130

**Excess entropy scaling for the segmental and global dynamics of polyethylene melts** — •Evangelos Voyiatzis, Michael Böhm, and Florian Müller-Plathe — Eduard-Zintl-Institut für Anorganische und Physikalische Chemie and Center of Smart Interfaces, Technische Universität Darmstadt, Alarich-Weiss-Strasse 4, D-64287 Darmstadt, Germany

The range of validity of the Rosenfeld and Dzugutov excess entropy scaling laws is analyzed for linear polyethylene chains. We consider two segmental dynamical quantities, the bond and the torsional relaxation times, and two global ones, the chain diffusion coefficient and the viscosity. The excess entropy is approximated by either a series expansion of the entropy in terms of the pair correlation function or by an equation of state for polymers. For all temperatures and chain lengths considered, the two excess entropy estimates are linearly correlated. The scaled segmental relaxation times fall into a non-linear master curve. For a fixed chain length, the reduced diffusion coefficient and viscosity scale linearly with the excess entropy. An empirical reduction to a chain length independent master curve is accessible for both quantities. The Dzugutov scheme predicts an increased value of the scaled diffusion coefficient with increasing chain length which contrasts physical expectations. The origin of this trend can be traced back to the density dependence of the scaling factors. In connection with diffusion coefficients and viscosities, the Rosenfeld scaling appears to be of higher quality than the Dzugutov. An empirical excess entropy scaling is also proposed which leads to a chain length-independent correlation.

## CPP 9: Nanoparticles and Composite Materials II (joint session CPP, BP)

Time: Monday 15:00–18:45 Location: C 243

CPP 9.1 Mon 15:00 C 243

**Do Macroscopic Properties of Nanocomposites Require Glassy Layers?** — Klaus Nusser and •Gerald J. Schneider — Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science & Institute of Complex Systems, 52425 Jülich, Germany

Inorganic/organic hybrid materials receive steadily growing interest due to their capability to show unprecedented properties. Most likely, at the length-scale of single chains, many different phenomena add and form the final material. Due to the small diameters, their specific surface area is very high, and thus may contribute significantly. To predict the material properties, many concepts have been developed to understand the influence of those chains close to surfaces. For example, a very common picture is the assumption of an immobilized or glassy layer when the polymer is very close to solid substrates.

In our contribution, we present macroscopic properties and show that these can be explained perfectly by the concept of a glassy layer. However, for these examples, our microscopic information by neutron scattering experiments evidence that the underlying assumptions are wrong, but our experiments permit a different explanation.

Based on our toolbox of hybrid materials, we used a well-defined system. As a consequence it allows us to formulate a theorem under which conditions new materials can be designed on the computer based on our results. Therefore, we believe that our achievements represent a major progress toward the prediction of macroscopic properties of nanocomposites based on information at the length-scale of a single chain.

CPP 9.2 Mon 15:15 C 243

**Dynamics of polymers in composites** — •Ulrich Scheler — Leibniz-Institut für Polymerforschung Dresden e.V.

Magnetic resonance is applied to study the dynamics of polymers interacting with inorganic solid surfaces. The dynamics of polymers over a wide range of correlation times is determined using magnetic resonance relaxation experiments for the investigation of systems in contact with solids and inorganic materials. In highly dispersed systems, these are nanoparticles coated with thin films have been investigated. Measurement of T2 or T1rho is ideally suited for the dynamics of chain segments, which is mostly affected by the interaction with the solid surface. Because of sensitivity issues only proton NMR signals have been detected. In order to obtain sufficient chemical resolution for instance to exclude solvent signals in swelling experiments high-resolution solid-state and NMR based on CRAMPS has been applied. These line narrowing techniques permit the selection or suppression of the solvent signal and thus one can focus on the polymer dynamics. It is seen, that there is much stronger motion and dynamics and putting the brushes compared to polymers of the same molecular weight. To investigate that further dedicated techniques for the selective excitations at the interface part based on magnetization transfer from the inorganic particle to the polymer has been applied. Spin-labels on polyelectrolytes permit the selective study of the dynamics of the polymer in the vicinity of the label. Because of the high sensitivity of EPR dynamics of individual layers in a multilayer system can be studied.

CPP 9.3 Mon 15:30 C 243

**Disentanglement in polymer-star mixtures** — •Hendrik Meyer — Institut Charles Sadron, CNRS UPR22, 67034 Strasbourg, France

We present a molecular dynamics simulation study of entangled melts mixed with particles of the order of the tube diameter. The choice of compact stars represents a model system of nanocomposites without polymer-particle adsorption. The particles remain well dispersed over the whole concentration range and the stars are sufficiently compact that the pure system is jammed. For this system, we observe a weak compression of the matrix chains with increasing volume fraction of stars. Short (unentangled) matrix chains get slowed down by adding particles to the system. When the matrix chains become significantly longer than the entanglement length, this trend is inversed and the matrix chains become faster because the particles dilute the entanglement network. The center-of mass (CM) dynamics exhibits regimes of anomalous diffusion in accordance with viscoelastic hydrodynamic interactions (VHI) [1]. At low and intermediate star-particles concentration, the particles themselves vary little in mobility, only at high concentration (above percolation), they become slowed down because of colloidal packing. As a result, the viscosity as a measure of the collective mobility drops when adding few particles to the melt because of disentanglement, and at high particle volume fraction the viscosity increases again because of colloidal caging. [1] J. Farago et al. PRL 107, 178301 (2011); PRE 85, 051807 (2012).

CPP 9.4 Mon 15:45 C 243

**Polymer/metal hybrids: Adhesion behaviour and polymer dynamics before and after corrosion treatment** — •Marieke Füllbrandt[1,2], Andreas Schönhals[2], and Regine von Klitzing[1] — [1]Technische Universitaet Berlin, Str. des 17. Juni 124, 10623 Berlin — [2]BAM Bundesanstalt fuer Materialforschung und -pruefung, Unter den Eichen 87, 12205 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. In a first step, the metal/polymer interface is characterized with regard to the adhesion behaviour on a macro- and microscopic length scale using contact angle (CA) measurements and colloidal probe atomic force microscopy. The latter method determines the adhesion force and energy which can be analysed and related to a work of adhesion per area. The effect of a (sub)micrometre scale roughness is considered using the Rabinovich approach. With CA measurements the surface energy of the solids is determined using the Owens-Wendt-Rabel-Kaelble method and further be related to the corresponding work of adhesion per area. In a second step, the influence of a corrosion treatment on the adhesion behaviour is investigated. Complementary, broadband dielectric spectroscopy measurements in a wide frequency (0.01 Hz to 1 MHz) and temperature range (-120 to 180 °C) are performed in order to characterize the polymer dynamics in bulk and at the metal interface before and after treatment.

CPP 9.5 Mon 16:00 C 243

**Organic inorganic hybrid PU-POSS networks: A multi-length-scale investigation of morphology and a multi-time-scale investigation of dynamics** — •Konstantinos N. Raftopoulos[1,2], Stefanos Koutsoumpis[3], Malgorzata Jancia[2], Konstantinos Kyriakos[1], Edyta Hebda[2], Christine M. Papadakis[1], Krzysztof Pielichowski[2], and Polycarpos Pissis[3] — [1]TU München, Physik-Department, Fachgebiet Physik weicher Materie, Garching — [2]Cracow University of Technology, Department of Chemistry and Technology of Polymers, Poland — [3]National Technical University of Athens, Department of Physics, Greece

Polyhedral oligomeric silsesquioxanes (POSS) bridge the gap between nanoparticles and conventional chemical reagents. A wide variety of organic, ligands bind on a sub-nm siliceous core, and allow it to participate as a nanobuilding block on the very structure of the macromolecular chain. Here, octa-OH functional moieties crosslink a phase separated polyurethane. On the basis of X-ray diffraction in a wide q-range covering both WAXS and SAXS and atomic force microscopy we show that POSS reside in the soft phase, and the hard microdomains become progressively thinner with increasing POSS content. The segmental dynamics of the soft phase slow down as a result of both crosslinking and diminishing microphase separation, as evidenced by differential scanning calorimetry and broadband dielectric spectroscopy. Interestingly, all the effects show a step-like behavior between 4 and 6 wt% of POSS, possibly as a result of a percolation of the POSS crosslinked phase.

CPP 9.6 Mon 16:15 C 243

**Nanomechanical Investigation of Rubber-modified Epoxy Resins** — •Lisa Maria Uiberlacker and Sabine Hild — Institute of Polymer Science, Johannes Kepler University, 4040 Linz, Austria

Epoxy resins have a broad application scope due to the wide range of properties which can be easily modified by mixing various basic components - e.g. to modify the toughness of epoxy resins rubber auxiliaries are added.

This study focused on epoxy mixtures based on a bisphenol A diglycidyl ether cured with diethyltoluenediamine with various amounts of nitrile rubber. Both, morphology and the mechanical properties of these two phase systems were examined with scanning force microscopy (SFM).

In SFM phase images the epoxy phase was clearly distinguished from the rubber phase. The nitrile rubber formed spherical domains in the epoxy matrix. Phase separation occurred also in the rubber matrix. Mechanical properties of both phases were quantified by nanoindentation experiments. In addition, the influence of different amounts of rubber additive on the toughness of the epoxy matrix was examined.

**15 min. break**

CPP 9.7 Mon 16:45 C 243

**Matryoshka-Doll-like Shish-Kebab Nanocomposite: Nanohybrid Shish-Kebabs within Nanofiber Shish-Kebabs** — •Matthias M.L. Arras[1], Richard Jana[1], Christian Grasl[2], and Klaus D. Jandt[1] — [1]Chair of Materials Science (CMS), Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Jena, Germany — [2]Center for Medical Physics and Biomedical Engineering, Medical University of Vienna, Austria

The shish-kebab morphology in semi-crystalline polymer fibers is a key to the outstanding properties of polymer fibers. Here, we present the creation of a two-level hierarchical fiber structure by combining two recent artificial shish-kebab nanostructures: The nanohybrid shish-kebab (NHSK), i.e., a carbon nanotube (CNT) overgrown by polymer kebabs and the nanofiber shish-kebab (NFSK), i.e., an electrospun nanofiber decorated by larger lamellae crystals. We tested the hypothesis that during electrospinning of a CNT/polymer solution the NHSK can form directly and that the resulting fibers can be used to subsequently create the NFSK. The resulting nanocomposite was analyzed by transmission and scanning electron microscopy and revealed the successful creation of both the NHSK and the NFSK. Thus, for the first time, we demonstrated the creation of the NHSK morphology during electrospinning. The two-level hierarchical nanocomposite is a proof of principle that the shish-kebab morphology can be extended from the nanoscale to the macroscale which may contribute to future high strength nanocomposites.

CPP 9.8 Mon 17:00 C 243

**Structural changes of diisocyanates covalently attached to the semiconducting carbon nanotube** — •Mariana Kozlowska[1], Jakub Goclon[2], and Pawel Rodziewicz[1] — [1]Institute of Chemistry, University of Bialystok, Poland — [2]Interdisziplinäres Centrum für Molekulare Materialien(ICMM) und Computer-Chemie-Centrum (CCC), Department Chemie und Pharmazie,Friedrich–Alexander–Universität Erlangen–Nürnberg

Reinforced polymers are of a great interest since the individual properties of the initial materials can be combined, resulting in a new hybrid material with better properties. Carbon nanotubes are popular polymer filler and reinforcing agent. They enhance the mechanical strength and corrosion resistance.

We performed first-principles DFT calculations of the covalent and noncovalent sidewall functionalization of metallic (6,0) and semiconducting (10,0) single-walled carbon nanotubes (SWCNTs) via the attachment of two aromatic diisocyanates: 4,4'-methylene diphenyl diisocyanate (MDI) and toluene-2,4-diisocyanate (TDI).

In this work, we focus on the structural rearrangements of the diisocyanates molecules covalently attached to the SWCNT(10,0) surface at the finite temperature, using the Car-Parrinello molecular dynamics (CP-MD) scheme.

Mariana Kozlowska is a beneficiary of the project Scholarships for PhD students of Podlaskie Voivodeship. The project is co-financed by European Social Fund, Polish Government and Podlaskie Voivodeship.

CPP 9.9 Mon 17:15 C 243

**Formation of anisotropic gold nanoparticles with different morphologies analysed by UV-Vis spectroscopy, SAXS and TEM** — •Tilo Schmutzler, Torben Schindler, Martin Schmiele, and Tobias Unruh — Friedrich-Alexander-University Erlangen-Nuernberg, Chair for Crystallography and Structural Physics, Staudtstrasse 3, 91058 Erlangen, Germany

Au nanoparticles (NPs) have been the subject of widespread research in the last two decades. Therefore, numerous studies dealing with the synthesis leading to exact shape and size control were made. Applications are expected in biological imaging, drug delivery and photothereapeutics.[1]

Especially anisotropic Au NPs show interesting optical behaviour due to their ability to absorb light at different wavelengths for more than one surface plasmon resonance. Via a modified seed-mediated growth synthesis route for gold nanorods[1] we were able to synthesize various morphologies of Au NPs with defined absorption bands (500-800 nm) in the UV-Vis spectrum and narrow distributions of the particle dimensions which could be determined by small angle X-ray scattering (SAXS) and transmission electron microscopy (TEM).

The particle formation of Au nanorods in contrast to other morphologies like star-like nanoaggregates under different conditions (temperature, concentration of precursors, ...) was investigated by UV-Vis spectroscopy, SAXS and TEM to understand indirectly the formation mechanism of such particles.

[1] C.J. Murphy et al., J. Phys. Chem B. 2005, 109, 13857-13870.

### CPP 9.10 Mon 17:30 C 243

**Local Chemical Characterization of Nanoporous Materials with Atom Probe Tomography** — •Carsten Nowak, Philipp Sauerbier, and Björn Pfeiffer — Georg-August-Universität Göttingen, Insitute for Materials Physics, Göttingen, Germany

Because of their high surface-to-volume-ratio and their chemical activity, nanoparticles and nanoporous materials receive a lot of interest in the areas of catalysis and electrochemistry. To obtain a detailed insight into reaction mechanisms, knowledge of the local chemical composition and structure, particularly at the surface of the material, is desirable.

Here we present experimental results on the local chemical characterization of nanoporous gold with atom probe tomography. The nanoporous gold with pore and ligament size of 50 nm, chosen as model system, is converted into a compact material by electron beam induced deposition of metalorganic precursors. Subsequently, the material is characterized with atom probe tomography which essentially is a combination of single molecule time of flight spectroscopy and atomic scale microscopy, thus allowing to characterize the local chemical composition of the filled material and particularly its former surface with sub-nanometer spatial resolution.

Although the preparation involves a chemical reaction of the surface with the precursor and thus alters the active surface of the nanoporous material, this approach offers the potential to detect chemical species at the surface of irregularly shaped nanoparticles with sub-monolayer sensitivity.

### CPP 9.11 Mon 17:45 C 243

**Semiconductor Nanocrystal Blinking monitored via Fast Spectrally and Intensity Resolved Single Molecule Spectroscopy** — •Clemens Göhler, Cornelius Krasselt, and Christian von Borczyskowski — Fakultät für Naturwissenschaften, TU Chemnitz, D-09126 Chemnitz

Colloidal CdSe Semiconductor Nanocrystals (NCs) are promising candidates for improving different applications, e.g. in photovoltaics or sensoring, due to their size-dependend optical and spectroscopic properties. With techniques from Single Molecule Spectroscopy, we avoid ensemble-averaging and investigate these characteristics on individual NCs. On that level, luminscence intermittency (so called blinking) is observable, for which the underlying mechanisms are yet not fully understood.

To contribute, we applied Change-Point-Analysis to time-correlated single-photon counts from single NC photoluminescence (PL) emission, which allows resolving discrete PL intensity levels [1]. In addition, we splitted the PL-signal with a dichroic beamsplitter towards two detectors. By combining these techniques, we were able to examine spectral diffusion within the single NC PL on a $\mu$s-timescale and to correlate that to the fluctuating emission intensity. The results are in agreement with blinking models based on a multiple recombination-center approach.

[1] Schmidt, R., Krasselt, C., Göhler, C., & von Borczyskowski, C. (2014). *ACS nano*, *8*(4), 3506-3521.

### CPP 9.12 Mon 18:00 C 243

**Interrelation of fluorescence and morphology of molecular aggregate structures** — •Mohammadreza Bahrami[1], Tamam Bohamud[1], Clemens Schindler[1], Lukas Rathje[1], Hannes Hartmann[1], J.A.A.W Elemans[2], Ingo Barke[1], and Sylvia Speller[1] — [1]University of Rostock, Institute of Physics, 18051 Rostock, Germany — [2]Radboud University Nijmegen, Institute for Molecules and Materials, 6525 AJ Nijmegen, The Netherlands

Metallo-porphyrins are widespread in nature and act as a key component in photosynthesis as well as in oxygen transport in blood cells. They have attracted much attention in view of applications like molecular wires, fluorescence switches, and light-energy conversion [1]. We study the spatially resolved photoluminescence from Copper-based porphyrin [2] aggregates as one of the deexcitation pathways of excitons. Among the different observed morphological motifs of the aggregates we here focus on branched strands with typical diameters of 50 - 100 nm. Fluorescence microscopy images show varying intensity along strands and junctions. In combination with atomic force microscopy we correlate fluorescence and structural properties to elaborate possible reasons of such morphology-dependent fluorescence. We further present fluorescence data on a composite system of silver nanostructures in the vicinity of molecule aggregates, and address the role of these metal systems as local sources of electromagnetic fields.

[1] Wenqi Zheng, et al., Dyes and Pigments 77 (2008) 153e157 [2] M.J.J. Coenen, et al., Phys. Chem. Chem. Phys. 15, 12451 (2013)

### CPP 9.13 Mon 18:15 C 243

**Electric detection of ortho and para water in fullerene cages** — •Benno Meier, Salvatore Mamone, Javier Alonso-Valdesueiro, Maria Concistrè, Andrea Krachmalnicoff, Richard J. Whitby, and Malcolm H. Levitt — School of Chemistry, University of Southampton, SO17 1BJ Southampton, United Kingdom

Water, like molecular hydrogen, exhibits spin isomerism, a phenomenon in which the entanglement of spatial and spin states leads to ortho and para spin isomers with different symmetry. The physical properties and the interconversion of the two isomers of molecular hydrogen are central to fields as diverse as astrophysics and nuclear magnetic resonance, but much remains unknown about the different isomers of water, owing to the difficulty of separating the two isomers. Here, we use fullerene cages to provide freely rotating water molecules at cryogenic temperatures in the form of the supramolecular endofullerene H2O@C60. Unlike molecular hydrogen, water has an electric dipole moment and we show that the dielectric constant, a bulk property, that is linked to the spin states via their molecular polarizabilities, changes upon ortho-para conversion that is induced by a sudden temperature change. Our findings are in excellent agreement with previous NMR studies and suggest the possibility to detect and eventually manipulate H2O@C60 molecules selectively depending on the nuclear spin state of the comprised water molecule.

### CPP 9.14 Mon 18:30 C 243

**Effective mechanical properties of graphene obtained by computational mechanical tests** — •Markus A. Hartmann[1], Melanie Todt[2], and Franz G. Rammerstorfer[2] — [1]Institute of Physics, Montanuniversität Leoben, 8700 Leoben, Austria — [2]ILSB, Vienna Institute of Technology, 1040 Vienna, Austria

Carbon nanostructures combine a high stiffness with low weight and an exceptional toughness making carbon a promising candidate for applications in structural mechanics. Understanding the mechanical properties of these structures on every length scale is of utmost importance to be able to exploit the full potential of these materials. In the presented work the effective mechanical parameters of graphene are assessed that are the necessary input parameters for large scale finite element calculations. Of special interest is the "effective thickness" in combination with the "effective Young's modulus" of monolayer graphene. Potentials obtained by ab initio calculations [1] were used in subsequent Monte Carlo simulations to assess the effective mechanical properties of graphene [2]. The membrane stiffness and the bending stiffness (and consequently the effective thickness) of graphene were evaluated. The results showed that the elastic modulus as well as the Poisson ratio corresponds well to values known from literature. For structures too small the continuum approximation breaks down and the effective thickness decreases, while it attains a constant value of approximately 0.132 nm for structures large than 5 nm.

[1] Holec et al., Phys. Rev. B 81, 235403 (2010)

[2] Hartmann et al., Europhys. Lett. 103, 68004 (2013)

# CPP 10: On-surface Polymerization

Time: Monday 15:00–17:45 Location: H 0105

**Invited Talk** CPP 10.1 Mon 15:00 H 0105

**Formation mechanisms of covalent nanostructures** — •Jonas Björk — Department of Physics, Chemistry and Biology, IFM, Linköping University, Linköping, Sweden

The on-surface reactions underlying the formation of covalent nanostructures are in many cases fundamentally different from their wet chemistry analogues. Furthermore, their mechanisms are often intractable from experiments due to short-lived intermediate and transition states, and to make use of the true potential of this approach we need to understand the factors controlling the on-surface reactions. Here, it will be demonstrated how density functional theory can be used as a powerful tool for gaining insight into the mechanisms of these reactions. Firstly, we will discuss the on-surface Ullmann coupling, where halogen-substituted molecules are used as the basic building blocks. The key aspects of this reaction scheme will be scrutinized for simple model systems, but we will also discuss the effect of increasing the complexity towards more realistic systems. In particular, it will be examined how metal adatoms affect the different reaction processes, as these have shown to play a pivotal role in experiments.

Secondly, we will briefly discuss the mechanisms of other coupling schemes presented during the last years, with focus on the homocoupling of terminal alkynes. This reaction has a completely different mechanism than that of the on-surface Ullmann coupling, with the coupling preceding the release of any side-products. Furthermore, the on-surface chemistry of alkynes is extremely rich, with several possible reaction products depending on molecule and/or surface.

**Invited Talk** CPP 10.2 Mon 15:30 H 0105

**Selective C-H Activation and C-C coupling on Metal Surfaces** — •Lifeng Chi — Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou 215123, P. R. China — Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Strasse 10, 48149 Münster, Germany

Selective C-H bond activation is one of the most interesting and challenging topics in chemical synthesis. Recently, the development of the *on surface chemistry* provides an alternative strategy for the C-H activations. In this talk an overview for C-H activation and the following C-C coupling on metal surfaces will be given, together with detailed report on alkane homo-coupling and aryl-aryl coupling via the C-H activation by introducing OH group in phenyl rings. The influence of metal surfaces on reaction activation and selectivity will be discussed.

**Invited Talk** CPP 10.3 Mon 16:00 H 0105

**On-Surface Synthesis on Insulating Substrates** — •Angelika Kuehnle — Physical Chemistry, University Mainz, 55099 Mainz, Germany

On-surface synthesis has attracted great attention in recent years due to its promising potential for creating functional structures directly on surfaces [1]. An exciting aspect of on-surface synthesis is the capability to arrive at thermally stable molecular structures that might not be accessible by solution chemistry. Using tailored building blocks allows for tuning the electron transport properties of the resulting structure. Especially the latter is of tremendous interest when considering future applications in the field of molecular electronics. Having molecular electronics applications in mind requires decoupling of the electronic structure of the molecular network from the underlying support surface. Thus, it is highly interesting to transfer on-surface synthesis strategies from metallic to insulating surfaces. In this talk, recent results in on-surface synthesis on an insulating substrate carried out in ultra-high vacuum are reported [2-4].

[1] A. Gourdon, Angew. Chem. Int. Ed. 47 (2008) 6950; [2] M. Kittelmann, P. Rahe, M. Nimmrich, C. Hauke, A. Gourdon, A. Kühnle, ACS Nano 5 (2011) 8420; [3] R. Lindner, P. Rahe, M. Kittelmann, A. Gourdon, R. Bechstein, A. Kühnle, Angew. Chem. Int. Ed. 53 (2014) 7952; [4] M. Kittelmann, M. Nimmrich, R. Lindner, A. Gourdon, A. Kühnle, ACS Nano 7 (2013) 5614

**15 min. break.**

**Invited Talk** CPP 10.4 Mon 16:45 H 0105

**On-surface polymerization - a synthetic route to 2D polymers** — •Markus Lackinger — Deutsches Museum, München, Germany — Technische Universität München, Physik Department, Garching, Germany

Flat surfaces appear to be the ideal template for the synthesis of regular 2D covalently cross-linked polymers. Surfaces can not only confine the reaction to two dimensions, but can also play an active chemical role during the polymerization. Hence, the material and crystallographic orientation of the surface can also be used to steer or even control the reaction. The main objective of the lecture is to critically discuss the status, the main challenges, and the potential of on-surface polymerization for the synthesis of 2D polymers.

Different coupling reactions were already employed in a surface-chemical approach, each with specific advantages and disadvantages. An important distinction is whether the reaction can be carried out under slightly reversibly conditions or necessarily remains fully irreversible. While polymerization close to thermodynamic equilibrium opens up ways to improved structural quality, purely kinetically controlled reactions apparently inevitably lead to highly defective networks. Using the example of on-surface Ullmann coupling a detailed view will be presented on the surface-dependence, possible reaction intermediates, and the relation between defects and kinetic reaction parameters. Finally, the potential of metastable intermediate organometallic networks to improve the structural quality of 2D polymers will be demonstrated.

**Invited Talk** CPP 10.5 Mon 17:15 H 0105

**On-surface azide-alkyne click chemistry and a novel metal-organic network based on Cu adatom trimers** — •Trolle Linderoth — Interdisciplinary Nanoscience Center (iNANO) and Department of Physics and Astronomy, Aarhus University, Denmark

Molecular nanostructures on solid surfaces are central to achieve advanced functional surfaces. Covalent synthesis with reactants adsorbed on surfaces has therefore been the focus of intense recent interest. In this context there is a need to identify suitable chemical reactions that will proceed under Ultra High Vacuum conditions. Early work in this direction from our group focused on the condensation reaction between aldehydes and amines to form imines [1-3]. Here, it was shown that the connectivity in two-dimensional surface polymeric networks could be controlled by kinetic parameters of the preparation procedure. More recently, we have explored the prototypical click-chemistry reaction of 1,3-dipolar Huisgen cycloaddition between azides and terminal alkynes to form a triazole product for reactants adsorbed on a Cu(111) surface (CuAAC reaction) [2]. Finally we have investigated the on-surface dehydrogenation reaction for tetra-hydroxy-benzene (THB) which enables formation of a novel metal-coordination network containing trimeric Cu-adatom clusters [3].

[1]: Angew. Chem. Int. Ed. 46 9227 (2007), Angew. Chem. Int. Ed. 47 4406 (2008).

[2]: J. Am. Chem. Soc, 135 2136 (2013).

[3]: Chem. Comm. 49, 9308 (2013), Angew. Chem. Int. Ed. 53 12995 (2014).

# CPP 11: Brownian Motion and Transport (joint session DY, CPP)

Time: Monday 15:00–18:45 Location: BH-N 243

**Invited Talk** CPP 11.1 Mon 15:00 BH-N 243

**universal statistics of records in random sequences** — •satya majumdar — cnrs, lptms, universite paris-sud, orsay, france

Records are rather common in everyday life: we are always talking of record rainfall, record temperature, records in sports and stock prices etc. When the random sequence consists of independent random variables, the record statistics is well known. In this talk, I'll discuss the record statistics in a strongly correlated random walk sequence and show that they are universal, i.e., independent of the noise (jump) distribution. Several applications and extensions will be discussed–such as the effect of a constant drift and the effect of measurement errors.

CPP 11.2 Mon 15:30 BH-N 243

**Three-dimensional Brownian motion of 3D-shaped particles** — •Felix Höfling — Max Planck Institute for Intelligent Systems, Stuttgart, and Institute for Theoretical Physics IV, Universität Stuttgart, Germany

The three-dimensional (3D) Brownian motion of colloidal particles of general 3D-shape is considered in the overdamped limit. First for an ellipsoidal particle, the Smoluchowski equation for the joint distribution of position and orientation is solved exactly through an expansion in moments. The non-Gaussian parameter is shown to simultaneously quantify the anisotropic positional diffusion and the orientational diffusion. The results are applied further to the interpretation of scattering experiments (e.g., dynamic light scattering) on suspensions of active (self-propelled) and passive nanoparticles.

Second, a screw-like shape, paradigmatic for chiral particles, is studied which gives rise to a strong hydrodynamic coupling between rotation and translation. Coupled Langevin equations for the six degrees of freedom are used to calculate auto- and cross-correlation functions of first and second order exactly. A suitable displacement–orientation correlation is shown to display a maximum at intermediate times, from which the strength of the rotation–translation coupling can be inferred. Finally, the above findings are generalised for a hydrodynamic friction matrix of general form, which encodes an arbitrary particle shape. The analytical results are supported by numerical simulations of the corresponding stochastic equations.

CPP 11.3 Mon 15:45 BH-N 243

**Velocity fluctuations of Brownian particle in inhomogeneous media and driven by colored noise as a sourse of 1/f fluctuations** — •Rytis Kazakevicius and Julius Ruseckas — Institute of Theoretical Physics and Astronomy, Vilnius University, A. Gostauto 12, LT-01108 Vilnius, Lithuania

Nonlinear stochastic differential equations generating signals with 1/f spectrum in a broad range of frequencies have been used so far to describe socio-economical systems [1]. We have derived such equation from Langevin equations that describe the motion of a Brownian particle in an inhomogeneous environment. The inhomogeneous environment can be a result of a linear potential affecting the Brownian particle together with the steady state heat transfer due to the difference of temperatures at the ends of the medium. The correlation of collisions between the Brownian particle and the surrounding molecules can lead to the situation where the finite correlation time becomes important, thus we have investigated the effect of colored noise in our model. Existence of colored noise leads to the additional restriction of the diffusion and exponential cut-off of the distribution of particle positions. Narrower power law part in the distribution of the particle positions results in the narrower range of frequencies where the spectrum has power law behavior.

[1] V. Gontis, J. Ruseckas and A. Kononovicius, Physica A, 389 100 (2010).

CPP 11.4 Mon 16:00 BH-N 243

**Hydrodynamically enforced entropic trapping of Brownian particles** — •Steffen Martens[1], Arthur Straube[2], Gerhard Schmid[3], Lutz Schimansky-Geier[2], and Peter Hänggi[3] — [1]Technische Universität Berlin, Berlin, Germany — [2]Humboldt-Universität zu Berlin, Berlin, Germany — [3]Universität Augsburg, Augsburg, Germany

In small systems spatial confinement causes entropic forces that in turn implies spectacular consequences for the control for mass and charge transport. Therefore, recent efforts in theory triggered activities which allow for an approximate description that involves a reduction of dimensionality. Up to present days, the focus was on the role of conservative forces and its interplay with confinement. Within the presented work, we overcome this limitation and succeeded in considering also "magnetic field" like, so termed non-conservative forces that derive from a vector potential [S. Martens et al., *Phys. Rev. Lett.* **110**, 010601 (2013)]. A relevant application is the fluid flow across microfluidic structures where a solute of Brownian particles is subject to both, an external bias and a pressure-driven flow. Then a new phenomenon emerges; namely, the intriguing finding of identically vanishing average particle flow which is accompanied by a colossal suppression of diffusion [S. Martens et al., arXiv:1407.5673]. This entropy-induced phenomenon, which we termed *hydrodynamically enforced entropic trapping*, offers the unique opportunity to separate particles of the same size in a tunable manner [S. Martens et al.,*Eur. Phys. J. ST* **222**, 2453-2463 (2013)].

CPP 11.5 Mon 16:15 BH-N 243

**On the Applicability of the Caldeira-Leggett Model to Condensed Phase Vibrational Spectroscopy** — •Fabian Gottwald, Sergei Ivanov, and Oliver Kühn — Institut für Physik University of Rostock, Rostock, Germany

Formulating a rigorous system-bath partitioning approach remains an open issue. In this context the famous Caldeira-Leggett (CL) model that enables quantum and classical treatment on equal footing has enjoyed popularity. Although this model is by any means useful as a theoretical tool, its validity for describing anharmonic dynamics of real systems is often taken for granted. We investigate the applicability of the model by comparing the spectra resulting from the Generalized Langevin dynamics that is based on the CL model, with their counterparts from explicit classical molecular dynamics. It is shown that the model is not able to describe real systems unless the system part of the potential is effectively harmonic. We demonstrate that it is this anharmonicity, that is at the core of all deficiencies of the model and also point out the mathematical origin of its breakdown.

**15 min. break**

CPP 11.6 Mon 16:45 BH-N 243

**Dynamics of stochatic resisitive switching** — •Paul Radtke[1], Arthur Straube[1], Andrew Hazel[2], and Lutz Schimanksy-Geier[1] — [1]Department of Physics, Humboldt-Universität zu Berlin, Berlin, Germany — [2]School of Mathematics, University of Manchester, Manchester, UK

Classes of dielectrics such as $TiO_2$ alter their resistance under the influence of an electric field or a current flowing through the system, an effect called resistive switching (RS). Thereby the resistance depends also on the past states of the system, it has a memory.

We will show how a particular one-dimensional lattice model for a bipolar device. In it, oxygen vacancies hop in between consequetive sites and thereby alter local resistances. Their dynamics governed by a Master equation with jumping rates modulated by an external electric field. We discuss the system properties and show that dynamics of the vacancies can be formulated in terms of a Burgers like equation. With its help the underlying motion of the oxygen vacancies is interpreted as nonlinear traveling waves.

CPP 11.7 Mon 17:00 BH-N 243

**Simulation of colloidal particles in channel geometries** — •Ullrich Siems and Peter Nielaba — University of Konstanz, Germany

This talk will present the results of Brownian Dynamics Simulations of colloidal particles in external fields confined in channels. Colloidal particles are well suited model-systems for a variety of problems on different length scales, ranging from gravitational collapses over the description of pedestrians to models for atomic sized problems. In such systems confinement into channels can have a great influence on the diffusion and transport properties.

CPP 11.8 Mon 17:15 BH-N 243

**Nonlinear Microrheological response to a step force** —

•Thomas Franosch — Institut für Theoretische Physik, Leopold-Franzens-Universität Innsbruck, Innsbruck, Austria

In a microrheological experiment the thermal or forced motion of a colloidal particle is monitored to obtain information on mechanical properties of the surroundings. While the linear response is well-characterized in terms of the fluctuation-dissipation theorem, few exact results are available for strong driving.

Here we consider the time-dependent velocity of a colloidal particle immersed in a dilute suspension of hard spheres in response to switching on a finite constant force. The dimensionless number quantifying the strength of the driving is the Péclet number $\mathrm{Pe} = F\sigma/k_B T$. We present an analytical solution exact to first order in the packing fraction. In particular, we show that at *finite times* the response is an analytic function of the Péclet number, but displays singular behavior for infinite times. Our solution technique extends the stationary state calculation [1] to the time-dependent case. The non-commutitavity of the limits $\mathrm{Pe} \to 0$ and time $t \to \infty$ is traced back to the long-time tail in the velocity-autocorrelation function due to repeated encounters with the same colloid. The scenario is strongly reminiscent of a driven particle in a lattice Lorentz model with frozen obstacles [2], and corroborates that linear response becomes qualitatively wrong at long times for arbitrarily small driving.

[1] T.M Squires and J.F. Brady, Phys. Fluids 17, 073101 (2005)

[2] S. Leitmann, T. Franosch, Phys. Rev. Lett. 111, 190603 (2013)

CPP 11.9 Mon 17:30 BH-N 243

### Enhancement of mobility in a feedback controlled 1D colloidal system with repulsive interactions

— •Robert Gernert and Sabine H. L. Klapp — Institut für theoretische Physik, Technische Universität Berlin

Feedback control schemes are a promising way to design static and dynamic properties of colloidal suspensions [1]. In the collective transport of colloids through 1D tilted washboard potentials clusters of attractive particles are known to overcome the hindering influence of the potential barriers [2]. Here we consider a corresponding system with repulsive interactions. To enhance the mobility we propose a feedback control scheme and demonstrate its function theoretically. The control is modelled by a symmetrically confining potential, like an optical tweezer, and it is always centered around the mean particle position. For the theoretical demonstration we use Dynamical Density Functional Theory (DDFT) with ultra-soft as well as hard-core particle interactions. For either type of interaction the influence of the hindering washboard potential can be suppressed completely – corresponding to an enhancement of the mobility by several orders of magnitude. Further, in the regime of moderate amplification velocity oscillations are induced.

[1] B. Qian, D. Montiel, A. Bregull, F. Cichos, and H. Yang, Chem. Sci. 4, 1420 (2013)

[2] M. Evstigneev, S. von Gehlen, and P. Reimann, PRE 79, 011116 (2009)

CPP 11.10 Mon 17:45 BH-N 243

### Surface interactions of active Janus particles on a hexagonal close-packed colloidal crystal surface

— •Udit Choudhury[1], John G. Gibbs[1,2], and Peer Fischer[1,3] — [1]Max Planck Institute for Intelligent Systems, Heisenbergstr. 3, 70569 Stuttgart, Germany — [2]Dept. of Physics & Astronomy, Northern Arizona University, Flagstaff, AZ 86011, USA — [3]Institute for Physical Chemistry, University of Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany

Autonomous, self-driven colloidal particles are being given greater attention in recent years due to the interesting dynamics associated with out-of-equilibrium systems. Although particle-particle interactions of active colloids, e.g. self-assembly and clustering, are beginning to be regularly studied, particle-surface interactions are less well investigated. Herein, we empirically study the surface interactions of spherical Janus-particles half-coated with Pt in the presence of hydrogen peroxide. The surface consists of close-packed 2D monolayer of hard spheres (beads). This non-planar surface thus corresponds to a periodic potential akin to a fcc (111) lattice face. In this way, the system is an analogue of surface diffusion of adatoms that possess kinetic energy. We find that as the concentration of hydrogen peroxide is increased, the effective translational diffusion also increases which is comparable to enhanced diffusion of adatoms on surfaces at higher temperatures. Rotational diffusion dictates fluctuations in the orientation of the driven bead that lead to jumps form one potential well to its nearest neighbor.

CPP 11.11 Mon 18:00 BH-N 243

### Charged transfer in a dynamical Landau-Zener Model: Application in QCA

— •Alejandro Santana-Bonilla[1], Mirna Kramar[1], Rafael Gutierrez[1,2], and Giovanni Cuniberti[1,2] — [1]Technische Universität Dresden Faculty of Mechanical Science and Engineering Institute for Materials Sciences — [2]Max Bergmann Center of Biomaterials

The development of molecular based quantum cellular automata (mQCA) would open the possibility to low-dissipation information processing. One key parameter in the mQCA paradigm is the stability of intra-molecular charge transfer, which guarantees the association of *1* and *0* to two different charge configurations in the mQCA building cell. Especifically, a given charge configuration needs to be stable against thermal fluctuations. Also important is how the mQCA charge state reacts to an external driver with a given time-dependence. In this study we present a theoretical study based on the solution of the time-dependent Schrödinger equation to describe intra-molecular charge transfer in an effective model of an mQCA cell under the action of a time-dependent driver field and including thermal fluctuations. The model is parametrized via first-principle calculations in a toy molecular system able to catch the minimal requirements of a m-QCA cell

CPP 11.12 Mon 18:15 BH-N 243

### Calibration free 3D tracking of confined nanoparticles in a tunable nanofluidic slit

— •Stefan Fringes, Michael Skaug, Heiko Wolf, Urs T. Dürig, and Armin W. Knoll — IBM Research, 8803 Rüschlikon, Switzerland

We investigate the behavior of nanoparticles in a nanofluidic slit with tunable confinement and spatial and temporal resolution of 10nm and 2ms, respectively. The high speed detection of the particles' X, Y and Z coordinates allows us to obtain the spatiotemporal probability distribution of individual particles and thus to study their confining potential-landscape both in lateral and vertical direction. To obtain the 3D trajectory of a nanometer-sized particle we use interferometric scattering detection (iSCAT). The method exploits the interference between the scattered wave from the particles and the highly reflective reference surface for a precise localization in vertical direction [1]. Evaluating the particle contrast for varying slit distances enables us to measure the scattering phase, amplitude, and consequently the z-position of individual particles without prior calibration of the particle contrast [2]. Precise knowledge of the nanoparticles' paths and surrounding potentials allows us to study confinement effects on Brownian motion and charge regulation at the participating interfaces. It further enables us to precisely trap and immobilize nanoparticles at a specific location on the substrate.

[1] P. Kukura et al., Nature Methods 6, 923-927 (2009).

[2] N. Mojarad et al., Optics Express 21, 8, 9377-9389 (2013).

CPP 11.13 Mon 18:30 BH-N 243

### Towards single molecule trapping and manipulation with dynamic temperature gradients

— Marco Braun, Andreas Bregulla, and •Frank Cichos — Molecular Nanophotonics Group, Universität Leipzig, Linnéstraße 5, 04103 Leipzig

Single nano-objects in solution are driven by Brownian motion which is fueled by thermal energy. These Brownian fluctuations increase in strength with increasing temperature. Therefore, it is at first glance counter intuitive to confine Brownian fluctuations with the help of elevated temperatures. In thermal nonequilibrium, however, temperature gradients induce thermo-phoretic and thermo-osmotic drifts which provide the means for single particle manipulation in solution. Here we describe experiments which use optically heated metal nanostructures to create dynamical temperature profiles in solution. These temperature profiles induce well defined thermo-phoretic drift fields and act as effective potentials for objects suspended in liquid. Combined with optical feedback mechanisms, such effective potentials can be shaped to store and manipulate single or even multiple objects in a small observation volume. The developed thermophoretic trapping system therefore paves the way for extended single molecule studies in solution or even well-controlled bi- or multi molecular interaction studies.

# CPP 12: Organic Thin Films

Time: Monday 15:00–19:30 Location: H 2032

**Invited Talk** CPP 12.1 Mon 15:00 H 2032

**Thin film growth studies using time-resolved X-ray scattering** — •Stefan Kowarik — Institut für Physik, Newtonstr. 15, 12489 Berlin

Thin film growth inherently is a non-equilibrium process. This means that the route to the final film structure is determined not simply by a minimization of the free energy, but by a non-trivial competition between thermodynamics and kinetics. For a quantitative understanding one therefore needs information on the nanoscopic surface processes such as molecular binding as well as surface diffusion and step-edge crossing. In situ X-ray scattering is ideally suited for such measurements as it can be used to monitor temporal changes on the atomic scale. We show how real-time in situ Grazing Incidence Small Angle Scattering (GISAXS) can be combined with simultaneous X-ray reflectivity measurements to characterize both in-plane and out-of-plane film structure as a function of time. While GISAXS gives information on nucleation densities and island sizes, reflectivity measurements make it possible to extract the out-of-plane density profile so that both measurements together give a rather complete morphological characterization. We give examples for growth of small-molecule organic semiconductors such as C60, where we determine diffusion barrier, step edge barrier and binding energy, but the techniques are equally applicable to growth of atomic systems. S. Bommel, N. Kleppmann, C. Weber, H. Spranger, P. Schäfer, J. Novak, S.V. Roth, F. Schreiber, S.H.L. Klapp, S. Kowarik, "Unravelling the multilayer growth of the fullerene C60 in real-time", Nature Communications 5, 5388 (2014).

CPP 12.2 Mon 15:30 H 2032

**Epitaxial Growth of a Methoxy-Functionalized Quaterphenylene** — •Frank Balzer[1], Roland Resel[2], Arne Lützen[3], Horst-Günter Rubahn[1], and Manuela Schiek[4] — [1]MCI, NanoSyd, University of Southern Denmark, Alsion 2, DK-6400 Sønderborg, Denmark — [2]Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria — [3]University of Bonn, Kekulé Institute for Organic Chemistry and Biochemistry, Gerhard-Domagk-Str. 1, D-53121 Bonn, Germany — [4]University of Oldenburg, Energy and Semiconductor Research Laboratory, Institute of Physics, Carl-von-Ossietzky-Str. 9-11, D-26111 Oldenburg, Germany

Thin films from conjugated small molecule semiconductors are important building blocks for organic electronics. Functionalization can control their electrical and optical properties, but also change thin film morphology. Here the epitaxial growth of a methoxy functionalized *para*-quaterphenylene (MOP4) on alkali halides as well as on mica is investigated by a combination of low energy electron diffraction (LEED), polarized (confocal) light microscopy (PLM), atomic force microscopy (AFM), and X-ray diffraction (XRD). On both substrates a thin film phase is present, resulting however in different morphologies: On the alkali halides mainly islands from upright molecules form, whereas on mica clusters and nanofibers from lying molecules grow. LEED even detects an initial wetting layer on mica with a different structure. Especially the fibers show a specific polarization pattern of the emitted blue fluorescence. Clusters and fibers age via Ostwald ripening due to water vapor, resulting in a strong change of morphology.

CPP 12.3 Mon 15:45 H 2032

**Influencing the growth of *para*-sexiphenyl through chemical tuning** — •Anton Zykov[1], Mino Sparenberg[1], Paul Beyer[1], Linus Pithan[1], Christopher Weber[1], Yves Garmshausen[2], Francesco Carlà[3], Stefan Hecht[2], Sylke Blumstengel[1], Fritz Henneberger[1], and Stefan Kowarik[1] — [1]Inst. f. Physik, Humboldt-Universität zu Berlin — [2]Inst. f. Chemie, Humboldt-Universität zu Berlin — [3]ESRF, Grenoble

We investigate the molecular growth of hybrid organic-inorganic semiconductor systems (HIOS) and show that chemical tuning can be used to optimize the growth mode [1]. We employ fluorination of *para*-sexiphenyl (6P) to drastically alter the growth mode from a rough three-dimensional towards a smooth, crystalline layer-by-layer growth as demanded for efficient opto-electronic devices with advanced properties. Our study combines *in situ* atomic force microscopy and *in situ* real-time X-ray scattering performed at the ID03 beamline at ESRF to monitor the evolution of the molecular thin film structure and morphology on non-polar ZnO (1010) substrates. In contrast to the parent molecule 6P, we observe for the fluorinated 6P a suppression of the growth of a second crystal phase and an increased molecular diffusivity together with a lower Ehrlich-Schwoebel barrier. As a consequence the interlayer mass transport is increased, which leads to the observed improvement in growth-mode.

[1] M. Sparenberg*, A. Zykov*, P. Beyer, L. Pithan, C. Weber, Y. Garmshausen, F. Carlà, S. Hecht, S. Blumstengel, F. Henneberger and S. Kowarik. *Phys. Chem. Chem. Phys.*, 2014, **16**, 26084-26093.

CPP 12.4 Mon 16:00 H 2032

**Negative thermal expansion based on collective rotational motions of PTCDI-C8 in a crystalline organic thin film** — •Sebastian Bommel[1,2], Linus Pithan[2], Christopher Weber[2], Gonzalo Santoro[1], Stephan V. Roth[1], Edgar Weckert[1], and Stefan Kowarik[2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Germany

The understanding of the structure-function relationship in molecular thin films for the fabrication of advanced functional nano-materials is still challenging because molecules possess many conformational and rotational degrees of freedom. Here we report on temperature-dependent rotation of the organic semiconductor PTCDI-C8. Highly crystalline organic thin films have been investigated using Grazing Incidence X-ray Diffraction (GIXD), which enables us to determine the temperature-dependent unit cell and the arrangement of molecules within the unit cell. From fitting the intensities of the Bragg reflections at different temperatures we find that the tilt angle of the molecules changes continuously with temperature and does not exhibit hysteresis. A change in molecular tilt of 4° is observed for a 200 K temperature difference. This collective mechanical response of a molecular rotation is connected with a large negative thermal expansion coefficient of the a-axis within the thin film unit cell of -135 ppm/K. Such negative thermal expansion offers highly desirable properties for the design of thermo-mechanical devices such as actuators.

CPP 12.5 Mon 16:15 H 2032

**Shape anisotropy of organic thin films induced by ion-beam irradiated rippled substrates** — •Markus Kratzer[1], Dominik Wrana[2], Konrad Szajna[2], Franciszek Krok[2], and Christian Teichert[1] — [1]Institute of Physics, Montanuniversitaet Leoben, Franz Josef Straße 18, 8700 Leoben, AUSTRIA — [2]Institute of Physics, Jagiellonian University, Lojasiewicza 11, 30-348 Krakow, POLAND

Control over thin film growth morphologies of conjugated molecules is a key issue in organic electronics. Here, we investigated the growth of the organic semiconductor para-hexaphenyl (6P) on ion bombarded, rippled $TiO_2(110)$ surfaces. Such substrates are highly anisotropic, representing one-dimensionally patterned templates with alternating ascending and descending step trains exhibiting typical step distances smaller 1 nm. 6P islands have been observed featuring clear shape anisotropy and discrete island widths according to the ripple wavelength. These observations are addressed to anisotropic detachment of molecules differently bound to the island rim at ascending and descending steps. A change of the average ripple length from ~11 nm to ~60 nm, resulted in a change of the average islands' length-to-width ratio from ~1.5:1 and ~4.5:1. In addition, strong diffusion anisotropy along and perpendicular to the ripples was found to be responsible for an increasing island density with decreasing ripple length.

**15 min. break.**

CPP 12.6 Mon 16:45 H 2032

**Thin film growth analysis of quinacridone on SiO2** — •Boris Scherwitzl and Adolf Winkler — Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria

Quinacridone (C20H12N2O2) is part of the group of H-bonded organic dyes with remarkable air stability and attractive semiconducting properties. The combination of inter- as well as intramolecular H-bonding with pi-pi stacking leads to highly crystalline film formations with unique charge transport behaviors. Understanding the initial growth, namely from the sub-monolayer regime up to a few layers, is a key factor in evaluating possible applications in future microelectronic devices. In this contribution, we report our recent efforts and studies on the initial growth behavior of thin quinacridone films on a silicon dioxide substrate under UHV conditions with respect to sample treatment. After preparing and analyzing the substrate surface with Auger Electron Spectroscopy, thin films were created via physical vapor deposition from a Knudsen cell and subsequently analyzed with Thermal Desorption Spectroscopy, Atomic Force Microscopy and Raman Spectroscopy. Both sputter cleaned samples and samples with a carbon layer on top were investigated and yielded similar results. It could be shown, that quinacridone films tend to form bulk-like structures bound by strong hydrogen bonds, even at sub-monolayer coverages. Furthermore, a comparison between metal Knudsen cell and glass evaporation source deposition was made.

CPP 12.7 Mon 17:00 H 2032

**Interface dipole and growth mode of partially and fully fluorinated rubrene on Au(111) and Ag(111)** — Falk Anger[1], Hendrik Glowatzki[2], Antoni Franco-Cañellas[1], Christoph Bürker[1], •Alexander Gerlach[1], Reinhard Scholz[3], Youichi Sakamoto[4], Toshiyasu Suzuki[4], Norbert Koch[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — [2]Helmholtz-Zentrum für Materialien und Energie GmbH, Berlin, Germany — [3]Institut für Angewandte Photophysik, TU Dresden, 01069 Dresden, Germany — [4]Institute for Molecular Science, Myodaiji, Okazaki 444-8787, Japan

Thin films of fully and partially fluorinated rubrene deposited on Au(111) and Ag(111) were investigated using ultraviolet and X-ray photoelectron spectroscopy [1]. We demonstrate that fluorination of the molecules is an efficient way for tuning the metal-organic interface dipole and the hole injection barrier [2,3].

Moreover, the results indicate that the pronounced electrostatic dipole moment of partially fluorinated rubrene ($F_{14}$-Rub) has a strong impact on the growth mode of these molecules. Most notably, we infer that the first layer of $F_{14}$-Rub on Au(111) and Ag(111) is formed by molecules with alternating orientation of their dipole moments, whereas the second layer shows a nearly uniform orientation.

[1] F. Anger et al., submitted
[2] F. Anger et al., Appl. Phys. Lett. **102** (2013) 13308
[3] M. Kytka et al., J. Chem. Phys. **130** (2009) 214507

CPP 12.8 Mon 17:15 H 2032

**Small organic molecules for stongly coupled microcavities** — •Felix Lemke, Vadim Lyssenko, and Karl Leo — Institut für Angewandte Photophysik, TU Dresden, Deutschland

Strongly coupled organic microcavities are a promising system to investigate exciton-polaritons. Due to their non-crystalline structure, the phonon-assisted relaxation to the $k = 0$ state is more probable than in inorganic microcavity systems. Even if organic materials are quite promising, small organic molecules showing strong coupling are very rare. The advantages are easier production procedures and long lifetimes.

An estimation of the usability for the investigated materials will be presented. Using absorption spectra and the Kramers-Kronig-Relation, the complex refractive index is calculated. By comparing these results with the cavity mode, already a first statement can be given. Further insight is gained with transfer matrix calculations. These calculations can also be used to optimise the coupling strength and therefore the splitting. The results are then compared to the measured data.

CPP 12.9 Mon 17:30 H 2032

**Magnetic transition metal phthalocyanine thin films: morphology, ordering, electronic structure and tuning of electronic properties via alkali metal doping** — •Olga Molodtsova[1], Sergey Babenkov[1], Karina Schulte[2], Volodymyr Maslyuk[3], Ingrid Mertig[3], Thomas Bredow[4], and Victor Aristov[1,5,6] — [1]DESY Hamburg, Germany — [2]MAX-lab Lund, Sweden — [3]Uni Halle, Germany — [4]Uni Bonn, Germany — [5]Uni Hamburg, Germany — [6]ISSP RAS, Russia

Magnetic transition metal phthalocyanines (MTM-Pc*s) are considered as materials for development of low dimensional molecular magnets, quantum computers and hybrid systems for memory devices. To make further progress in development such devices both the understanding and the tailoring of the physical, chemical and transport properties of the organic semiconductor components are required. The evolution of electronic structure of the MTM-Pc*s intrinsic and with potassium doping has been studied by means of photoemission spectroscopy, near-edge X-ray absorption fine structure and DFT calculations. The DFT calculations and detailed analysis of the core-level spectra permit us to suggest possible lattice sites for the potassium ions. The data disclosed filling of the lowest unoccupied molecular orbital upon doping and associated changes of the core level absorption spectra. None of the films prepared in our studies showed a finite electronic density of states at the Fermi level. Acknowledgements: This work was supported by the RFBR Grant No. 13 -02-00818 and the BMBF-Project No. 05K12GU2, PSP-Element No. U4606BMB1211

CPP 12.10 Mon 17:45 H 2032

**Cross-linking-induced disappearance of surface-enhanced Raman scattering in aromatic self-assembled monolayers** — •André Beyer[1], Marcel Mainka[1], Xianghui Zhang[1], Thomas Huser[2], and Armin Gölzhäuser[1] — [1]Physics of Supramolecular Systems, University of Bielefeld, 33615 Bielefeld, Germany — [2]Biomolecular Photonics, University of Bielefeld, 33615 Bielefeld, Germany

Surface-enhanced Raman scattering (SERS) spectra from aromatic self-assembled monolayers (SAMs) were recorded with the assistance of gold nanoparticles in different geometries. SAMs on planar gold surfaces with gold nanoparticles on top as well as SAMs on gold nanoparticles yielded comparable spectra with high signal-to-noise ratios. The cross-linking of aromatic SAMs by electron exposure results in the formation of carbon nanomembranes (CNMs). We demonstrate the formation of CNM-shells due to electron exposure of SAM-covered gold nanoparticles. Surprisingly, no Raman scattering in the range between 200 – 3100 $\text{cm}^{-1}$ was detectable from any aromatic SAM after cross-linking in the different SERS detection geometries. This finding was supported by performing SERS measurements on CNM/SAM samples which yielded no signal from the CNM but an intense signal from the SAM. Implications, possible mechanisms, and potential applications of this effect will be discussed.

**15 min. break.**

CPP 12.11 Mon 18:15 H 2032

**High-speed confocal Raman imaging of carbon nanotubes** — •Michael Ludemann, Susanne Hartmann, Anne-D. Müller, and Falk Müller — Anfatec Instruments AG, Melanchthonstr. 28, D-08606 Oelsnitz (V)

Raman spectroscopy is a powerful tool in terms of chemical analysis and determination of physical properties. The ability of scanning the sample during a measurement provides an insight into these properties in a spatially resolved way by converting spectral features into color code images.

Due to a huge number of image points, Raman mapping is seriously affected by long acquisition times. A new Raman spectrometer is designed for excellent coupling to an atomic force microscope (AFM) with the focus of maximized light throughput. Here, the optimum compromise for a sufficiently high signal-to-noise ratio is achieved at 8 ms exposure time per pixel resulting in an image acquisition time of less than 3 minutes, even with a non-cooled CCD. Based on this development, high-speed Raman mapping measurements on carbon nanotube (CNT) bundles on a silver/glass substrate are presented.

Raman mapping of single CNTs enables to distinguish between different types of CNTs. The spatial distribution of the CNT bundles and hot spot induced surface enhanced Raman spectroscopy (SERS) will be presented, as well.

CPP 12.12 Mon 18:30 H 2032

**Fast IR laser mapping ellipsometry for the study of functional organic thin films** — •Andreas Furchner[1], Guoguang Sun[1], Helge Ketelsen[2], Jörg Rappich[3], and Karsten Hinrichs[1] — [1]Leibniz-Institut für Analytische Wissenschaften – ISAS – e. V., Schwarzschildstraße 8, 12489 Berlin, Germany — [2]SENTECH Instruments GmbH, Schwarzschildstraße 2, 12489 Berlin, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium-Photovoltaik, Kekuléstraße 5, 12489 Berlin, Germany

The infrared spectral range provides information about the structural and chemical properties of functional organic thin films. The need to characterize these properties with high lateral resolution in short measurements times requires a new generation of infrared ellipsometer. A novel laboratoy-based infrared laser mapping ellipsometer is presented that allows for measurements with lateral resolutions of 0.12 mm and time resolutions down to 80 ms per spot. The ellipsometer is applied for the optical characteriztion of inhomogeneous poly(3-hexylthiophene) and poly($N$-isopropylacrylamide) organic thin films used for opto-electronics and bioapplications.

CPP 12.13 Mon 18:45 H 2032

**Characterization of advanced biomaterials for the medical device industry using Synchrotron Radiation-based FTIR microspectroscopy and X-Ray spectroscopic techniques** — •Andrea Hornemann[1], Beatrix Pollakowski[1], Bonnie Tyler[2], Gerald Holzlechner[3], Anna Belu[4], Arne Hoehl[1], and Burkhard Beckhoff[1] — [1]Physikalisch-Technische Bundesanstalt, Berlin, Germany — [2]National Physics Laboratory, London, United Kingdom — [3]BAM Federal Institute of Materials Research and -Testing, Berlin, Germany — [4]Medtronic, Minneapolis, U.S.A.

Since its early development implantable medical devices had tremendous impact on the quality of life. But still today many implants cause inflammations due to incompatibility with human tissues or due to device related infections. Hence, there is a need for exploring new advanced biomaterials that comprise thin film coatings, surface grafted biomolecules, nanoparticle coatings, drug-eluting films, and especially bioresorbable components. Reliable metrological tools for the rapid characterization of medical devices are essential to probe their physicochemical properties. Both vacuum-based and ambient techniques, represented here by X-ray and FTIR spectroscopic techniques, allow for a characterization of surface layers, contaminants on the surface of medical devices in the manufacturing environment, and enable the detection of defects and chemical constituents in the near-surface region. The measurement sequences exhibit the potential of the use of orthogonal methods as FTIR and X-ray spectrometry to significantly contribute to the traceable and reliable characterization of medical devices.

CPP 12.14 Mon 19:00 H 2032

**Molecular Orientations in Photochromic Layers on Silicon**(111) **Investigated by X-ray Absorption Spectroscopy** — •Daniel Przyrembel[1], Michael Åxman Petersen[2,3], Andreas Hebert[2], Karola Rück-Braun[2], Cornelius Gahl[1], and Martin Weinelt[1] — [1]Department of Physics, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Department of Organic Chemistry, Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany — [3]Department of Chemistry, Danmarks Tekniske Universitet, Anker Engelunds Vej 1, 2800 Kongens Lyngby, Denmark

Fulgimides are a class of photochromic molecular switches that undergo ring closing and opening upon illumination with UV and visible light, respectively.[1] When coupled to self-assembled monolayers (SAMs) of suitable anchoring molecules they retain the ability to reversibly isomerize and show photostationary states dominated by either a ring-opened $E/Z$ mixture or the ring-closed form.[2] We have investigated individual preparation steps towards as well as the resulting densely packed SAMs of a fulgimide on Si(111) single crystal surfaces by X-ray absorption spectroscopy. From the polarization-dependent contrast of the near edge X-ray absorption fine structure (NEXAFS) we deduced mean molecular orientations with respect to the sample surface and we evaluated the changes induced by UV illumination.

[1] Y. Yokoyama *Chem. Rev.* **2000**, *100*, 1717-1739.
[2] K. Rück-Braun, M. Å. Petersen, F. Michalik *et al. Langmuir* **2013**, *29*, 11758-11769.

CPP 12.15 Mon 19:15 H 2032

**Nucleation of Vaterite-Phase Calcium Carbonate by Poly Glutamic Acid Peptides on Gold** — •Hao Lu, Matthew A. Hood, Rafael Muñoz-Espí, Mischa Bonn, and Tobias Weidner — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Nature uses proteins and peptides containing acidic residues to control the crystal structure of polymorph materials such as calcium carbonate. Among the three most typical anhydrous polymorphs - calcite, aragonite and vaterite - the latter is the most thermodynamically unstable phase, and occurs rarely as biomineral. However, the vaterite structure can be stabilized in vitro by the presence of soluble biomolecules. Previous studies have focused on nucleation in the solution phase. Here we demonstrate interfacial nucleation: vaterite can be stabilized by specifically designed peptides bound to inorganic substrates. As a model system, we used a thiol-terminated poly glutamic acid sequences attached to a gold surface. The data show that the adsorbed peptides act as effective templates for the crystallization of a vaterite film. Using several complementary surface analytical techniques we follow structural changes of the peptide structure induced by the crystallization, which provides molecular-level insights into the biomineralization process of calcium carbonate.

## CPP 13: Focus: Field Controllable Functional Polymers II

Time: Monday 15:00–18:30 Location: C 264

CPP 13.1 Mon 15:00 C 264

**Multiscale Finite Element Modeling of Magnetoactive Materials** — •Philipp Metsch, Christian Spieler, and Markus Kästner — Institute of Solid Mechanics, Technische Universität Dresden, 01062 Dresden, Germany

Magnetorheological elastomers feature mechanical moduli that become strongly enhanced by an applied external magnetic field as well as the ability to generate magnetically induced deformations and mechanical actuation stresses. Typically, these materials represent a two-component system, in which micron-sized magnetizable particles are embedded in a cross-linked polymer network. Since the effective material behavior of magnetorheological elastomers is essentially determined by the constitutive properties of the individual components and their geometrical arrangement in the composite, this contribution will apply a homogenization approach for coupled magneto-mechanical problems. Starting from the properties of the magnetizable particles and the polymeric matrix, a weakly coupled model based on a continuum formulation of the problem is presented.

The governing equations are solved using the extended finite element method that allows the use of non-conforming, structured meshes which do not have to be adapted to the particle-matrix interfaces. This is advantageous if complex systems representing stochastic and structured particle distributions are considered. The obtained results are compared to those from other modeling approaches and experimental investigations.

CPP 13.2 Mon 15:15 C 264

**Theoretical study of Janus-like magnetic particles at low temperature** — •Ekaterina Novak[1], Elena Pyanzina[1], and Sofia Kantorovich[1,2] — [1]Ural Federal University, Lenin av. 51, 620000, Ekaterinburg, Russia — [2]University of Vienna, Sensengasse 8, 1090, Wien, Austria

Application of complex innovation methods in the field of magnetic materials led to a synthesis of magnetic Janus particles [Zhao and Gao, Adv. Mat., 2009; Smoukov et al., Soft Matter., 2009]. The two faces of magnetic Janus particles are the magnetic and nonmagnetic hemispheres. Applying an external electric or magnetic field one can assemble such magnetic Janus particles in staggered chains, chain-like or mesh-like superstructures and double and staggered chains. Driving the rotations of such colloids opens new perspectives in biomedical and technological applications. Here we present a theoretical study of Janus-like magnetic particles at low temperature. We would aim at investigating only one possible dipolar orientation and use the shift of the dipole, which in Janus particles correspond to the size of the magnetic side, as a control parameter to investigate both ground state structures and thermodynamically equilibrium self-assembly. To describe the basic features of the Janus-type magnetic colloids, we put forward a simple model of a spherical particle with a dipole moment shifted outwards the centre and oriented perpendicular to the particle radius. Using direct calculations and molecular dynamics computer simulations, we investigate the ground states of small clusters and the behaviour of bigger systems at low temperature.

CPP 13.3 Mon 15:30 C 264

**Magnetic gels - The influence of the sample shape on the deformation behaviour** — •Rudolf Weeber and Christian Holm — Institut fuer Computerphysik, Allmandring 3, 70569 Stuttgart

Magnetic gels are hybrid materials, consisting of magnetic particles immearsed in a hydrogel or elastomer. They are of interest due to the intricate interplay between elastic and magnetic forces observed in them. For example, magnetic gels can change their elasticity and shape, when an external magnetic field is applied. This property makes them interesting for applications in medicine and engineering.

It has been shown that two mechanisms exist by which a magnetic gel can deform in a homogeneous magnetic field. The first one is present only in magnetic gels in which the magnetic particles act as the cross-linker. It relies on a coupling of the orientation of the magnetic nanoparticles to the polymer matrix. The second mechanism, which will be the focus of this contribution, is based on the change of the average dipole-dipole interaction between the nanoparticles as they align to an external field.

Here, we discuss a recently developed coarse-grained simulation model for magnetic gels to study this deformation mechanism. It allows us to examine both, the influence of the local configuration of magnetic nanoparticles and the shape of the entire gel sample on the material's deformation in an external magnetic field.

CPP 13.4 Mon 15:45 C 264

**Magneto-Sensitive Elastomers** — •Sahbi Aloui and Manfred Klüppel — German Institute of Rubber Technology, Hannover, FRG

Magneto-sensitive elastomers (MSE) consist of a non-magnetic polymer matrix in which magnetic filler particles are embedded. These adjustable materials are able to ensure adaptability to changing environmental conditions by varying in-operando their dynamical properties. MSE have proven themselves in several practical applications like adaptive vibration control systems, a recently patented sensor for temperature measurements and industrial adhesives.

We study the non-linear dynamical-mechanical behavior and the magnetorheological response of MSE. Considerable influences on the properties of the MSE exert the magnetic fillers. Basic parameters like filler volume fraction in the prepared MSE, chemical composition and size distribution of magnetic particles play a major role. We focus on an optimization of mechanical and magnetic properties of MSE by preparing an anisotropic MSE, whose stiffness and hysteresis behaviors show magnetic orientation dependence. Combining highly reinforcing magnetic nanoparticles with micro-sized particles is advantageous to obtain a MSE with high switch ability in a magnetic field and reasonable mechanical properties.

References Aloui S., Klüppel M. *Magneto-Rheological Response of Elastomer Composites with Hybrid-Magnetic Fillers*, Smart Materials and Structures (submitted) Karl C., McIntyre J., Alshuth T., Klüppel M., Kautsch. Gummi Kunstst. 66/1-2 (2013), 46-53

**Invited Talk** CPP 13.5 Mon 16:00 C 264

**Magnetic particles in polymer harness: Modeling mesoscopic magnetomechanics of polymer composites** — •Yuriy Raikher[1,2] and Oleg Stolbov[1,2] — [1]Institute of Continuous Media Mechanics, Ural Branch of RAS, Perm, 614013, Russia — [2]Perm National Research Polytechnic University, Perm, 614990, Russia

Weakly-linked rubber-like materials filled with micron-size multi-domain grains are nowadays considered as the most technologically desirable media. They are sufficiently soft elastically and sufficiently loaded magnetically as to display strong magnetomechanical effects like field-induced strains, tuning of the elastic modulus, etc. In now discussed and tested applications of these soft magnetic elastomers (SMEs), a usual working element is a 3D sample. Here we consider SME films, which are more flexible mechanically and, thus, more sensitive to the field than the 3D ones. The macroscopic behavior of a SME film comes out as a net result of the particle-matrix interaction. In such samples, the particle displacements crucially depend on the direction of the applied field. Moreover, in the numerical modeling, we use, instead of the customary dipole-dipole potential, another one, which much better accounts for the magnetic softness of the multi-domain particles. The field-induced response of SME films at the mesoscopic scale is discussed and projected to the macroscopic observations. Support by RFBR grants 13-01-96056 and 14-02-96003 and project MIG S26/617 from the Ministry of Education and Science of Perm Region are acknowledged.

CPP 13.6 Mon 16:30 C 264

**Influence of the dipole moment orientation inside particles on the macroscopic behaviour of magnetic ellipsoids systems** — Anna Gudkova and •Elena Pyanzina — Ural Federal University, Lenin av. 51, Ekaterinburg, 620000, Russia

Magnetic anisotropic particles in the last years became an independent fast-emerging branch of dipolar soft matter research. In this contribution we focus our attention on the magnetic ellipsoids, which have 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). The theoretical study and results of computer simulations for microstructure and magnetic, rheological and structural properties for the systems with different dipole orientation and particle anisotropy are presented. It was shown that all aforementioned characteristics strongly depend on the particle anisotropy and the dipole orientation as well as external magnetic field. As a result one can drastically change macroscopic responses of the systems. 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 13.7 Mon 16:45 C 264

**Interplay between thermo-mechanical and functional properties of inductively heated nanomagnetite filled shape-memory polymers** — •Kazakeviciute-Makovska Rasa and Steeb Holger — Ruhr-Universität Bochum Universitätsstr. 150 D-44780 Bochum

One of the main problems in development of thermo-responsive shape-memory polymer (SMP)-based devices for engineering and medical applications is the design of a safe and effective method of thermal actuation. The conventional method of actuation involves the direct heating. A novel alternative to this method is the inductive heating. This may be achieved by the addition of ferromagnetic particles to a polymer matrix and exposing SMPs to an alternating magnetic field to cause the volumetric and remote heating. Based on the data available in open literature, we discuss the bulk thermo-mechanical and functional properties and performance of nanomagnetite reinforced SMPs. The analysis includes a wide range of filler parameters, induction parameters, and filler distribution configurations with the aim to understand the effects of particle size and shape on the thermal, pseudo-elastic, and rheological properties of this class of SMP nanocomposites. A parallel analysis of the functional behavior of nanomagnetite reinforced shape memory polymers is concerned with the shape fixity and shape recovery properties as well as the maximum recovery stress.

**15 min. beak**

CPP 13.8 Mon 17:15 C 264

**Branched structures in dipolar hard sphere fluids: junctions revisited.** — •Sofia Kantorovich[1,2], Alexey Ivanov[2], Lorenzo Rovigatti[1], Jose Maria Tavares[3], and Francesco Sciortino[4] — [1]University of Vienna, Vienna, Austria — [2]Ural Federal University, Ekaterinburg, Russia — [3]University of Lisbon, Lisbon, Portugal — [4]University of Rome "La Sapienza", Rome, Italy

To clarify the scenario of temperature-induced structural transitions in magnetic nanocolloids of moderate concentrations we developed a theoretical approach and performed an extensive Monte Carlo simulations study. Our theoretical approach is based on the density-functional theory, where single nanoparticles can self-assemble in primary "defect-free" chains and rings as well as in "defect structures" in which primary structures are merged with the help of specific "defect particles". We are able to limit the amount of possible branching points (defects) to three main types, using a thorough numerical and visual analysis of simulation results (Rovigatti et al., J. Chem. Phys., 2013). The defects of types X and Y are serving as cross-linkers between primary structures, whereas defect of type Z could only appear within chains and rings. One of the key findings here is that at high dipolar strength (very low temperature) all Y defects are to be replaced by more energetically advantageous and infinitesimally magnetoresponsive defect structures made of two rings cross-linked by X defect (in contrast to the predictions of Tlusty and Safran, Science, 2000).

CPP 13.9 Mon 17:30 C 264

**Equilibrium behavior of ferromagnetic supramolecular brushes** — •Pedro A. Sánchez[1], Joan J. Cerdà[2], Tomás Sintes[2], and Sofia S. Kantorovich[1,3] — [1]University of Vienna, Sensengasse 8, 1090, Wien, Austria — [2]Instituto de Física Interdisciplinar y Sistemas Complejos (UIB-CSIC), E-07122 Palma de Mallorca, Spain — [3]Ural Federal University, Lenin av. 51, Ekaterinburg, 620000, Russia

We present our recent progress on the characterization of the equilibrium structural behavior of ferromagnetic supramolecular brushes. These systems consist of a polymer brush-like structure formed by grafted supramolecular ferromagnetic filaments instead of molecular polymers. In general, magnetic filaments are obtained by crosslinking magnetic colloids by means of macromolecules to form a permanent magnetoresponsive chain structure. The grafting of magnetic filaments on surfaces is a promising strategy to create field controllable coatings with many potential applications.

Our study is focused on the determination of the dependence of the brush structure on the interplay between the steric repulsions and the magnetic interactions of the colloids, and is based on extensive molecular simulations and analytical theories.

CPP 13.10 Mon 17:45 C 264

**The study of the diffusion coefficient in the magnetic fluids: theory and computer simulation** — •Alla Muratova[1] and Sofia Kantorovich[1,2] — [1]Ural Federal University, Lenin av. 51, 620000, Ekaterinburg, Russia — [2]University of Vienna, Sensengasse 8, 1090, Vienna, Austria

We present the results on the mobility and diffusion coefficients in the systems of magnetic dipolar particles. Of course, 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 consider the ferrofluids with chain aggregates of dipolar spheres. In our study, we combine theoretical approach and computer simulation. In theoretical study, we use Density Functional Approach to obtain the chain concentrations. Then we can calculate the mobility and diffusion coefficients. We know that the self-diffusion coefficient decreases with growing particle volume fraction and dipole-dipole magnetic interaction parameter in the three-dimensional samples of magnetic fluids. In this case, we have good agreement between the theory and computer simulation. So we can expand our theory to the cases of bidisperse ferrofluids and magnetic fluids with geometrical constraints. Thus, we study how the mobility and diffusion coefficients depend on the system polydispersity, granulometric composition, geometrical constraints and dipolar stregths.

CPP 13.11 Mon 18:00 C 264

**Dynamic mechanical response of dielectric elastomer actuators for the control of optical elements** — •Gunnar Gidion, Matthias Kollosche, Werner Wirges, and Reimund Gerhard — Applied Condensed-Matter Physics, Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Straße 24-25, 14476 Potsdam-Golm, Germany

Dielectric Elastomer Actuators (DEA) consisting of an elastomer membrane with compliant electrodes are investigated with respect to their voltage-induced dynamic mechanical response. The in-plane deformation of prestretched acrylic and silicone membranes in a rectangular frame is captured with a high-speed camera and analysed with respect to the frequency response of the device. The geometry is examined for different pre-stretches at frequencies of up to 300 Hz. The AC driving voltage is applied in combination with various DC-bias voltages. The results are compared to the shear moduli obtained by means of dynamic mechanical analysis (DMA) of the respective materials. In addition, it has been observed that the sinusoidal electrical excitation is not translated into a purely sinusoidal motion of the actuator membrane. This observation is discussed in terms of viscoelastic creep and harmonic distortion. The results can be used to understand and modify the dynamic electromechanical response of soft actuators for optical applications such as e.g. the control of the grating period in soft diffractive optical elements.

CPP 13.12 Mon 18:15 C 264

**Tuning elastomer membranes: Materials design and electrical stability of acrylic and silicone elastomers** — •Matthias Kollosche[1], Martin Blümke[2], Gunnar Gideon[1], Miriam Biederman[2], Hartmut Krüger[2], and Reimund Gerhard[1] — [1]Institute of Physics and Astronomy, Universitiy of Potsdam, Potsdam, Germany — [2]Fraunhofer Institute for Applied Polymer Research Fraunhofer IAP, Potsdam, Germany

Soft dielectrics are sensitive to multiple stimuli, such as changes in e.g.temperature or pH value, and to control parameters such as mechanical stretch or electrostatic pressure. The latter two mechanisms are employed in Dielectric Elastomer Actuators (DEAs) - capacitors that consist of an elastomer sandwiched between two compliant electrodes. Many researchers have focused on the optimization of dielectric-elastomer and conductive-electrode materials with particular emphasis on higher permittivities, lower elastic compliances, and higher electric-breakdown strength as well as on high electrode conductivities and stretchability. Nevertheless, the stability and the durability have not yet been studied in detail. Here soft dielectric materials such as the industrial acrylic (3M, VHB 4905) and silicone (Wacker, Elastosil) elastomers are compared to specifically modified silicones with enhanced permittivity and reduced stiffness. The resulting transducers are characterized without and with pre-stretch over relatively long periods of time and under high electric fields. Results will be discussed in terms of durability and failure mechanisms of the materials under investigation for possible use in advanced elasto-optical devices.

## CPP 14: Crystallization, Nucleation and Self Assembly II (joint session CPP, DY)

Time: Monday 15:45–18:30 Location: PC 203

CPP 14.1 Mon 15:45 PC 203

**Estimation of crystal nucleation barriers from Monte Carlo simulations** — •Antonia Statt[1,2], Peter Virnau[2], and Kurt Binder[2] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz,Staudinger Weg 9, 55128 Mainz, Germany — [2]Graduate School of Excellence Materials Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany

A fluid in equilibrium in a finite volume V with particle number N at a density exceeding the onset density of freezing may exhibit phase coexistence between a crystalline nucleus and surrounding fluid. Using a method suitable for the estimation of the chemical potential of dense fluids we obtain the excess free energy due to the surface of the crystalline nucleus. There is neither a need to precisely locate the interface nor to compute the (anisotropic) interfacial tension [1]. As a test case, a soft version of the Asakura-Oosawa model [2] for colloid polymer-mixtures is treated. While our analysis is appropriate for crystal nuclei of arbitrary shape, we find the nucleation barrier to be compatible with a spherical shape, and consistent with classical nucleation theory.

[1] A. Statt, P. Virnau and K. Binder, PRL 2014 (in press)

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

CPP 14.2 Mon 16:00 PC 203

**Nano-Dewetting in Colloidal Crystal Drying** — •Mulda Muldarisnur and Frank Marlow — MPI für Kohlenforschung, 45470 Mülheim an der Ruhr, Germany

The drying of colloidal crystals is connected with a continuous shrinkage process [1]. However, several minutes after starting the drying, the system seems to take a breath before it shrinks monotonously until its final state after about one day. This short period we call "v"-event because of the shape of the curve characterizing the lattice constant: a decrease followed by a counter-intuitive increase which ends after one hour. This event is found in time-dependent optical spectra. It is assigned to the start of a nano-dewetting process occurring at the colloidal particles.

[1] M. Muldarisnur and F. Marlow, Observation of Nano-Dewetting in Colloidal Crystal Drying, Angew. Chem. Int. Ed. 2014, 53 (33), pages 8761-8764

CPP 14.3 Mon 16:15 PC 203

**Solidification fronts in supercooled liquids: how rapid fronts can lead to disordered glassy solids** — •Andrew Archer[1], Morgan Walters[1], Uwe Thiele[2], and Edgar Knobloch[3] — [1]Department of Mathematical Sciences, Loughborough University, Loughborough, LE11 3TU, UK — [2]Westfälische Wilhelms-Universität Münster, Institut für Theorestische Physik, Wilhelm-Klemm-Str. 9, 48149 Münster, Deutschland — [3]Department of Physics, University of

California at Berkeley, Berkeley, CA 94720, USA

We determine the speed of a crystallization/solidification front as it advances into the uniform liquid phase after it has been quenched into the crystalline region of the phase diagram, for systems of soft particles. We calculate the front speed by assuming the system can be treated using dynamical density functional theory (DDFT). There are two mechanisms by which the front can advance, depending on whether the liquid state is linearly stable or not. When linearly unstable, the front speed can be calculated by applying a marginal stability criterion. As the solidification front advances, the density profile behind the advancing front develops density modulations, whose wavelength $\lambda$ is a dynamically chosen quantity. For shallow quenches, $\lambda$ is close to that of the crystalline phase and so well-ordered crystalline states are formed. However, when the system is deeply quenched, $\lambda$ can be quite different from that of the crystal, so the solidification front naturally generates disorder in the system. Significant rearrangement and aging must subsequently occur for the system to form the regular well-ordered crystal that corresponds to the free energy minimum.

**Invited Talk** CPP 14.4 Mon 16:30 PC 203

**Spontaneous symmetry breaking in 2D: Kibble-Zurek mechanism in colloidal monolayers at finite cooling rates** — Sven Deutschländer, Georg Maret, and •Peter Keim — Universität Konstanz

The Kibble-Zurek mechanism describes the evolution of defects and domains when a system is forced through a phase transition with spontaneously broken symmetry. It describes Higgs field in the early universe shortly after the Big Bang or condensed matter systems like quenched quantum fluids. For a system with second order phase transition, the domain structure naturally arises when it is cooled at a finite rate. Since diverging correlation length are accompanied with critical slowing down, the system has to fall out of equilibrium for any non-zero rate; At this so called fall out time the correlation length is frozen out before the transition can take place globally. Within this picture, we investigate the non-equilibrium dynamics in a soft-matter analogue, a two-dimensional ensemble of colloidal particles which in equilibrium obeys the Kosterlitz-Thouless-Halperin-Nelson-Young melting scenario with continuous phase transitions. The ensemble is exposed to finite cooling rates of the pair-interaction parameter (being an inverse system temperature) at very different rates from deep in the isotropic fluid into the polycrystalline phase. We analyse defect configurations as well as the evolution of orientationally ordered domains quantitatively via video microscopy and show that their frozen-out length scale follows an algebraic decay as function of the quench rate as predicted by the Kibble-Zurek mechanism.

**15 min. break.**

CPP 14.5 Mon 17:15 PC 203

**Molecular Dynamics Study of Colloidal Quasicrystals** — •Heiko G. Schoberth, Heike Emmerich, and Thomas Gruhn — Lehrstuhl für Material- und Prozesssimulation, Universität Bayreuth, D-95440 Bayreuth

Quasicrystals are of continuous interest due to their fascinating fundamental properties and their potential applications like advanced photonic materials. In the last years colloidal quasicrystals have been found in solutions with spherical polymer core-shell micelles [1]. Fundamental aspects have been investigated in theoretical studies in which the core-shell micelles are represented with a step-potential, in which the core-core interaction is modeled by infinite repulsion while the shell-shell interaction is modeled by a plateau at constant height $\epsilon$ and width $\lambda$ [2]. The real interaction of the micelles is a continuous function which is more smeared out at the core and shell boundaries. Therefore, we perform coarse-grained molecular dynamics simulations to investigate the influence of the potential shape on the self-assembling structure. Varying the parameters we study systematically the phase diagram finding domains with 6-,10-,12-,24-fold symmetries. With increasing smoothness of the potential the phase diagram changes qualitatively and the geometry of the phase boundaries gets more regular.
[1] Fischer S. et al., PNAS, 108, 1810-1814 (2011)
[2] Dotera T. et al., Nature, 506, 208-2011 (2014)

CPP 14.6 Mon 17:30 PC 203

**Real-time study of multi-step nucleation in protein crystallization** — •Andrea Sauter[1], Felix Roosen-Runge[2], Fajun Zhang[1], Gudrun Lotze[3], Robert M. J. Jacobs[4], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]Institut Laue-Langevin, Grenoble, France — [3]European Synchrotron Radiation Facility, Grenoble, France — [4]Department of Chemistry, University of Oxford, UK

We present a real-time study of protein crystallization of bovine $\beta$-lactoglobulin in the presence of the divalent salt $CdCl_2$ using SAXS and optical microscopy. Monitoring the crystallization kinetics, we demonstrate a multi-step crystallization mechanism particularly focusing on the role of the metastable intermediate phase (MIP). In the first step, an intermediate phase is formed, followed by the nucleation of crystals within the intermediate phase. In the next step, this intermediate phase is consumed by nucleation and slow growth and the crystals are exposed to the dilute phase. At this stage, the number of crystals stays nearly constant, whereas the crystals grow rapidly due to access to the free protein molecules in the dilute phase. The results suggest that increasing the salt concentration near the transition zone *pseudo-c*** reduces the energy barrier for both the MIP and crystal nucleation. The observed kinetics can be well described using a rate-equation model based on a clear physical multi-step picture. This real-time study not only provides direct evidence for a multi-step process for protein crystallization, but also elucidates the role and the structural signature of the MIP in the non-classical process of protein crystallization.

CPP 14.7 Mon 17:45 PC 203

**All-atom MD simulation of fullerene dyads in water: Exploring hydrophobic hydration** — •Olga Guskova[1], Srinivasa Rao Varanasi[1,2], and Jens-Uwe Sommer[1,3] — [1]Leibniz-Institut für Polymerforschung Dresden e. V., Theorie der Polymere, Hohe Str. 6, 01069 Dresden, Deutschland — [2]University of Queensland, School of Chemical Engineering, St Lucia QLD 4072, Australia — [3]Technische Universität Dresden, Institut für Theoretische Physik, Zellescher Weg 17, 01069 Dresden, Deutschland

The nanometer-sized C60 fullerene, being a boundary case between small and large hydrophobes, represents an interesting object for the investigation of hydrophobic hydration. Extensive MD simulations are performed to study the solvation of pristine fullerene and fullerene dyads as well as their self-assembly in water [1]. The solute-solvent interactions, which reflect in the structure of solvation shells, translational and orientational dynamics of water molecules near the hydrophobic C60 cage and hydrophilic side chain, the H-bond networks and their defects, as dangling -OH bonds, are described. The agglomeration behavior of fullerenes is evaluated by determining sizes of the clusters, solvent accessible surface areas, and shape parameters. [1] O. Guskova, S.R. Varanasi, and J.-U. Sommer, J. Chem. Phys. 141 (14), 144303 (2014).

CPP 14.8 Mon 18:00 PC 203

**Phase field simulations of particle capture during directional solidification of photovoltaic silicon** — Heike Emmerich[1], •Henning Hörstermann[1], Julia Kundin[1], Jochen Friedrich[2], Maral Azizi[2], Christian Reimann[2], Arne Cröll[3], Thomas Jauss[3], and Tina Sorgenfrei[3] — [1]University Bayreuth, Chair of Material and Process Simulations, Bayreuth, Germany — [2]Fraunhofer IISB, Erlangen, Germany — [3]University Freiburg, Institute for Geosciences, Freiburg, Germany

We study the interaction between the solidification front and SiC particles present in the melt during the growth process of silicon for solar cells. Particles of a given size are pushed in front of the interface for growth velocities below a critical value and are incorporated into the crystal for growth velocities above this value. The existing theoretical models for particle capture find a relationship between critical particle size and critical growth velocity by assuming an equilibrium between a combination of gravity, drag, lift and other forces acting on the particle in the vicinity of the interface. For silicon these models predict significantly higher critical particle sizes than observed in experiments. We use a phase field model to test if these deviations can be explained by deviations from the spherical particle shape usually assumed in the theoretical models or effects like the deformation of the interface caused by the presence of the particle. In addition to testing and adapting existing theories, we narrow down the possible underlying mechanisms by identifying relevant length scales and other properties that are required to explain the experimental results.

CPP 14.9 Mon 18:15 PC 203

**Crystallization kinetics in printed active layers for organic solar cells** — •Stephan Pröller[1], Feng Liu[2], Chenhui Zhu[3], Peter Müller-Buschbaum[4], Thomas P. Russell[2], Alexander Hexemer[3], and Eva M. Herzig[1] — [1]Technische Universität München, Munich School of Engineering, 85748 Garching, Germany — [2]University of Massachusetts Amherst, Department of Polymer Science and Engineering, MA 01003 Amherst, Massachusetts, USA — [3]Lawrence Berkeley National Laboratory, Advanced Light Source, CA 94720 Berkeley, California, USA — [4]Technische Universität München, LS Funktionelle Materialien, 85748 Garching, Germany

Organic solar cells are a promising alternative to silicon based inorganic ones. Among other advantages like high absorption, a key advantage is the processability out of solution. This allows for printing of large area photovoltaic devices at low costs at low energy input. The morphology and crystalline properties of the active layer is of utmost importance for the functionality like exciton separation or charge carrier transport and thus for the performance of the produced devices. So far, not much is known on the crystallization kinetics of printed organic photoactive layers. Using an industrial slot-die printing process we studied the morphology evolution of a photoactive blend by in-situ X-ray scattering methods. With these experiments we are able to picture the process of crystallization of the polymer blend. We identified different stages during crystallization and propose a model for the crystal growth. This understanding is important to gain control over the morphology development of the system to improve organic solar cell performance.

## CPP 15: P1: Interfaces and Thin Films

Time: Monday 16:00–19:00 Location: Poster A

CPP 15.1 Mon 16:00 Poster A

**Study of contraction/spreading of microdroplets** — •Tak Shing Chan[1,2], Joshua D. McGraw[1], Simon Maurer[1], Thomas Salez[3], Michael Benzaquen[3], Elie Raphaël[3], Karin Jacobs[1], and Martin Brinkmann[1,2] — [1]Saarland University, Saarbrücken, Germany — [2]Max-Planck institute, Göttingen, Geermany — [3]ESPCI, Paris, France

A non-equilibrium liquid drop sitting on a smooth substrate will contract or spread depending on the microscopic contact angle and the initial shape of the drop. Previous studies assume a huge separation of length scales between the drop size R and the slip length b, as a result the drop remains as a spherical cap and interface deformations due to viscous effects are localized in a small region near the contact line . A well-known example is a drop spreading over a completely wetting surface, which follows Tanner*s law. In this project, we both experimentally and theoretically investigate contraction/ spreading of micro-droplets in the regimes where these two length scales are not far separated. Instead of a quasi-static shape during the evolution, the profiles display more structures in these regimes.

CPP 15.2 Mon 16:00 Poster A

**Investigations on ZnO scattering layers for OLED applications** — •Lorenz Biessmann, Christoph J. Schaffer, Johannes Schlipf, Volker Körstgens, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85738 Garching

By now the internal quantum efficiency of organic light-emitting diodes (OLEDs) reached values close to 1 but the overall efficiency still suffers on the extraction of the photons from the device. For further improvements of the performance one can apply a scattering layer to the device. Besides the direct structuring of the substrate surface, the attachment of a transparent layer on the substrate is a very promising approach. With an optical band gap of 3.3 eV, ZnO is a suitable material for this method. In this work ZnO is used as an additional layer on a glass substrate to achieve scattering abilities. For this purpose a structure giving diblock copolymer template was combined with sol-gel chemistry for tailoring the ZnO scattering layer. This yields thin films with nano- and micro-structures. The film morphology as probed by scattering techniques and SEM is related to the spectral response to gain a structure-function relationship.

CPP 15.3 Mon 16:00 Poster A

**Monte Carlo Simulation of Thin Film Polymer Melts** — •Andre Galuschko[1], Michael Lang[1], Torsten Kreer[1], and Jens-Uwe Sommer[1,2] — [1]Leibniz Institute of Polymer Research Dresden, Hohe Straße 6, 01069 Dresden, Germany. — [2]Institute of Theoretical Physics, Technische Universität Dresden, Zellescher Weg 17, 01062 Dresden, Germany.

We present Monte Carlo simulation data on conformations and dynamics of polymer melts confined in narrow slits of different widths and compare with data of bulk systems. We find that in confined geometries the chains swell laterally, they retain and even expand their spatially long-range correlations as compared to bulk polymers and in contrast to the assumption of a complete screening of excluded volume. Long chains in bulk melts show entangled dynamics with a clear signature of a $t^{1/4}$-power law for the mean square displacements of innermost monomers at intermediate time scales. This behavior is gradually lost by confining the melts in slits with decreasing width. For ultra-thin films, the dynamics appears to follow a $t^{1/2}$ dependence over the entire sub-diffusive regime. However, the terminal relaxation time is significantly increased as compared to Rouse relaxation. This interesting observation was not reported previously and is the focus of our ongoing research.

CPP 15.4 Mon 16:00 Poster A

**Molecular dynamics simulation of the interaction of polyamines with silica substrates** — •Sergii Donets, Arezoo Dianat, Rafael Gutierrez, Manfred Bobeth, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany

The role played by organic components in the process of biosilicification, resulting in well-defined three-dimensional silica structures in algae, has not been completely clarified. Especially in the case of diatoms several organic components have been meanwhile identified, including silaffins, silacidins, and polyamines. In this study we perform classical and quantum molecular dynamics simulations addressing two major issues related to polyamines: 1) the possible protonation states and protonation sites in short polyamines, and 2) the interaction of differently protonated polyamines with silica surfaces in order to identify the possible molecular conformations in dependence on the degree of protonation. Our results are in good quantitative agreement with results based on NMR experiments.

CPP 15.5 Mon 16:00 Poster A

**Structural investigation of ferrocene containing polymers in thin films and at the liquid/air interface** — •Haiko Didzoleit[1], Markus Gallei[2], Johannes Elbert[2], Matthias Rehahn[2], and Bernd Stühn[1] — [1]TU Darmstadt, Experimental Condensed Matter Physics — [2]TU 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 poly(ferrocenylsilane)- poly(vinyl pyridin) PFS-P2VP) and their structural properties at liquid/air and solid/air interfaces. These films are prepared as Langmuir monolayers on a water substrate and as Langmuir-Blodgett multilayer films on a solid silicon substrate. The structural properties are monitored by X-Ray reflectivity in situ (water subphase) and ex situ (silicon substrate) and analysed in terms of standard models.

The structure of the Langmuir monolayer is dominated by the P2VP block partner and strongly ruled by the surface pressure in the monolayer. Besides their structural changes the ferrocene moiety can be reversibly switched from diamagnetic to paramagnetic state by oxidation/reduction. We determine the magnetic properties of thin films by SQUID magnetometry. The oxidised state induces a conformational change leading to a swelling of the polymer film on solid substrates and to increasing solubility in water. The impact of these external variables on the structural properties will be shown for different composites of the diblock copolymer.

CPP 15.6 Mon 16:00 Poster A

**Simultaneous Mapping of Long-Range Attractive Forces and Near-Surface Interaction Forces with Multi-Set point Intermittent Contact (MUSIC) Mode AFM** — •Diana Voigt, Eike-

Christian Spitzner, and Robert Magerle — Technische Universität Chemnitz, Chemnitz, Germany

Studies using intermittent contact (IC) mode atomic force microscopy (AFM) often focus on imaging the surface morphology and on understanding contrast formation due to the mechanical response of the specimen. Here we study the contribution of long-range interactions, such as electrostatic and van der Waals interactions, as well as local differences in hydrophobicity using MUSIC mode AFM. Substrates partially covered with self-assembled monolayers either with carbon or amine terminated tail groups are studied. This mimics protein surfaces with locally different degrees of hydrophobicity. We aim at a detailed understanding of long-range and near-surface tip-sample interactions under different conditions. A methodological point of interest is the question about the ability to measure the different interactions in one single-pass measurement using MUSIC mode AFM.

CPP 15.7 Mon 16:00 Poster A

**Accurate Refractive-Index Determination from First- and Second-Order Critical Angles of Periodic Surface Patterns** — •Christoph Meichner[1], Lothar Kador[1], Andreas Schedl[2], Hans-Werner Schmidt[2], Christian Neuber[2], and Klaus Kreger[2] — [1]University of Bayreuth, Institute of Physics and Bayreuth Institute of Macromolecular Research (BIMF), 95440 Bayreuth, Germany — [2]University of Bayreuth, Macromolecular Chemistry I and Bayreuth Institute of Macromolecular Research (BIMF), 95440 Bayreuth, Germany

We present a novel method for the determination of the refractive-index dispersion of transparent solid films. The approach is based on irradiating collimated monochromatic light onto the sample with the illuminated spot carrying a periodic surface pattern. A simple rotational stage is sufficient for measuring critical angles of the light propagating in the film. From these angles, the refractive indices are calculated. To study the accuracy of our method, we prepared samples of a PDMS cast resin (*Sylgard*® 184) and compared the results to those obtained with an Abbe refractometer. The data are in good agreement, considering the angular resolution of the stage and the precision of the grating constant.

CPP 15.8 Mon 16:00 Poster A

**Ultrafast structural dynamics of membrane-bound water molecules revealed by two-dimensional surface-specific vibrational spectroscopy** — •Ruth Livingstone[1], Zhen Zhang[1], Lukasz Piatkowski[2], Huib J. Bakker[2], Mischa Bonn[1], and Ellen H. G. Backus[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]FOM Institute AMOLF, Science Park 104, 1098 XG Amsterdam, The Netherlands

We explore the structure and structural dynamics of water in contact with a model lipid membrane (a DPTAP monolayer) using ultrafast time-resolved 2-dimensional sum-frequency generation spectroscopy. With this highly surface-specific technique we monitor the ultrafast frequency fluctuations of the O-H stretch vibrations, that directly reflect the structural dynamics of the water hydrogen-bonding network. For water interacting with a lipid membrane the frequency correlations decay on a sub-picosecond timescale. This timescale does not change upon isotopic dilution of the water, revealing that the fast spectral dynamics are not the result of Förster energy transfer, as previously observed at the water-air interface, but rather result from ultrafast fluctuations in the local hydrogen-bonding network of membrane-bound water molecules.

CPP 15.9 Mon 16:00 Poster A

**Optical Tracking of Single Ag Clusters in Nanostructured Water Films** — •Stefan Krause, Martin Hartmann, Ingolf Kahle, Martin Neumann, Mario Heidernätsch, Stefan Spange, and Christian von Borczyskowski — Technische Universität Chemnitz

Beside organic fluorescent molecules inorganic nano particles have attracted increasing attention as optical probes for soft matter during the past two decades. Especially the photo stability of inorganic materials makes them suitable as fluorescent labels and nano probes. Thereby the fluorescence of a single particle serves as a sensitive probe for its environment and changes of the fluorescence lifetime, emission wavelength, polarization and position can report spatial and temporal heterogeneities in the environment of the particles which are not accessible with ensemble methods. Here we report on the spatial diffusion of single silver nano clusters of the size of about one nano meter within structured water layers on pure SiO2. The diffusion reveals a twofold spatial heterogeneity of the water films. The interaction of water molecules with the surface results in an *ice-like* structuring of the first 2 to 3 mono layers while higher layers exhibit an unstructured, *water-like* formation of the molecules. In addition, irregularities in the density of surface silanols which can be influenced by different surface treatment processes leads to formation of lateral islands. As a result of this structuring diffusion shows immobile, slow and fast diffusing clusters. This experiment provides insights into the processes of water film formation and its heterogeneities.

CPP 15.10 Mon 16:00 Poster A

**Interfacial melting of ice confined in layered sheet silicates** — •Hailong Li[1], Julian Mars[1], Johannes Grosse[1], Thomas Buslaps[2], and Markus Mezger[3,1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]European Synchrotron Radiation Facility, Grenoble, France — [3]Johannes Gutenberg-Universität Mainz, Germany

Most of the fresh water on earth is stored in the form of ice. Ground ice and permafrost contain 3 times more fresh water than all the lakes. The material properties of these permafrost composites strongly depend on the molecular scale structure of the ice/solid interface. Early in 1859, Faraday proposed the existence of a liquid-like layer at ice surfaces. Interfacial melting at well-defined single crystalline ice/solid interfaces was studied by x-ray reflectivity and other techniques. However, the understanding of the interfacial melting of ice and the structure of the liquid-like layer is still under debate. Layered sheet silicates such as exfoliated vermiculite are ideal materials to study the interfacial melting of ice in a geologically relevant system. We employ high-energy x-ray diffraction to measure the temperature dependence of the crystalline ice fraction in ice/vermiculite composites with a high interface to volume ratio. From the anisotropy of the ice reflections in textured samples with aligned vermiculite sheets we extract the preferred orientation of the confined ice crystals.

CPP 15.11 Mon 16:00 Poster A

**Influence of adhesion on composite mechanical and electric properties of thin Poly(3-hexylthiophene-2,5-diyl) (P3HT) films on stiff substrate (ITO electrode on glass) by means of AFM Force Distance Curves (FDC) and conductive AFM** — •Dorothee Silbernagl[1], Christiane Weimann[1], and Heinz Sturm[1,2] — [1]BAM Federal Institute for Materials Research, Berlin, Germany — [2]Technical University Berlin IWF, Berlin, Germany

Mechanical properties of thin polymer films on stiff substrates have been investigated by AFM FDC and are known to be a composite of the properties of both materials. The contribution of each material to the resulting module depends primarily on film thickness. Films act as mechanical "insulator" with regard to the substrate[Si1]. The additional influence of adhesion between film and substrate has been demonstrated: the higher adhesion the better mechanical properties are "conducted", increasing the influence of substrate's mechanical properties on composite module[Si2]. We propose an analogy between the mechanical conductivity and the electric conductivity which can be exploited to quantify the influence of the adhesion. Conductive polymer films (P3HT) on a substrate/electrode (glass/ITO) have been measured using AFM FDC and conductive AFM. For this purpose spin coated films of P3HT (30nm<t<150nm)on ITO substrates have been aged to induce partial delamination. Film properties and their changes due to aging have been monitored by confocal Raman spectroscopy.
[Si1] Silbernagl, Cappella. Surface Science, 2009, 603(16),2363-2369.
[Si2] Silbernagl, Sturm, Cappella. Langmuir, 2009, 25(9),5091-5097.

CPP 15.12 Mon 16:00 Poster A

**Shape and Wrinkle Analysis of deflated Elastic Capsules** — •Jonas Hegemann, Sebastian Knoche, and Jan Kierfeld — TU Dortmund, 44221 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 15.13 Mon 16:00 Poster A

**Influence of the chemical structure on the slip boundary condition of liquids** — •Mischa Klos[1], Sebastian Backes[1], Juan Manuel Castillo Sanchez[2], Hans Hasse[2], and Karin Jacobs[2] — [1]Saarland University, Experimental Physics, D-66123 Saarbrücken — [2]TU Kaiserslautern, Laboratory of Engineering Thermodynamics, D-67663 Kaiserslautern

On small scales, especially in microfluidic devices, the role of the solid/liquid interface gets more important for the flow dynamics. Our experiments probe slippage via the dewetting 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 exhibit slip lengths up to micrometers [2]. On AF1600, no significant slip is observed . Scattering studies reveal an ordering of the PS side chains at the solid/liquid interface depending on the structure of the substrate [3]. Recent simulations were able to characterize the used SAMs[4]. However, the situation changes if PMMA or polyvinylpyridine (PVP) are used: Dewetting experiments show that slip is less pronounced in PVP and in PMMA films. Obviously, the structure of the side groups play a significant role. X-ray reflectometry supplement this hypothesis and give further insight to the slippage mechanism at the solid/liquid interface. [1] O. Bäumchen, et.al., J Phys Condens Mat 24 (2012) 325102 [2] R. Fetzer, et. al, Europhys Lett 75 (2006) 638 [3] P. Gutfreund, et. al.,Phys Rev E 87 (2013) 012306 [4] J.M. Sanchez, et. al. submitted

CPP 15.14 Mon 16:00 Poster A

**Molecular scale structures of ionic liquid interfaces under electric potential** — •Julian Mars[1], Peter Reichert[1], Kasper Skov Kjaer[2], Tim Brandt van Driel[2], Martin Meedom Nielsen[2], Moshe Deutsch[3], and Markus Mezger[1,4] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Centre for Molecular Movies, Department of Physics, TechnicalUniversity of Denmark, Lyngby, Denmark — [3]Department of Physics and Institute of Nanotechnology andAdvanced Materials, Bar-Ilan University, Ramat-Gan, Israel — [4]Johannes Gutenberg-Universität Mainz, Germany

Electrolyte interfaces under electric potential are of a great scientific and technological interest. For diluted electrolyte solutions, the interfacial ion profile can be described by the Gouy-Chapman theory. However, for solvent-less electrolytes such as ionic liquids the diluted solution approximation is clearly invalid. Despite of their importance, the molecular scale structure of ionic liquids near electrodes is still under debate. We have studied the potential dependent interfacial structure of room temperature ionic liquids with high-energy x-ray reflectivity and impedance spectroscopy measurements. We find oscillatory charge density profiles consisting of alternating anion- and cation-enriched layers at both cathodic and anodic potentials. This structure is shown to arise from the same ion-ion correlations dominating the liquid bulk structure. The relaxation dynamics of the interfacial structure were studied by impedance spectroscopy and time resolved x-ray reflectivity experiments with sub-millisecond resolution.

CPP 15.15 Mon 16:00 Poster A

**Alginate - Chitosan Multilayer Films and Their Properties** — •Hakan Kaygusuz[1,2], F. Bedia Erim[2], and Regine von Klitzing[1] — [1]Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Strasse des 17. Juni 124, D-10623 Berlin, Germany — [2]Department of Chemistry, Istanbul Technical University, 34469 Maslak, Istanbul, Turkey

Alginate and chitosan are oppositely charged polysaccharides, being anionic and cationic, respectively. These polysaccharides have many uses, both crosslinked and uncrosslinked. Negatively charged surfactant, sodium dodecyl sulfate (SDS), has effects on viscosity and mechanical properties of linear and crosslinked alginate structures. For example addition of SDS decreases the viscosity of the alginate solutions and increases the Young's modulus of crosslinked alginate gels. Therefore it is aimed to observe the ability of forming multilayer films with these materials and the effect of SDS on the film structure.

Multilayers of these polyelectrolytes were prepared using dip-coating method. The properties such as film thickness and roughness were characterized using ellipsometry, atomic force microscopy and X-ray reflectometry. The effect of sodium chloride and sodium dodecyl sulfate concentration, and the number of double layers on film properties were observed. The crosslinking and swelling ability of these films were discussed.

## CPP 16: Organic Electronics and Photovoltaics: Transport of Charges - from Molecules to Devices (joint session with HL, TT)

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

CPP 16.1 Tue 9:30 C 130

**Electronic properties of biphenylene and the biphenylene carbon sheet** — •Johann Lüder, Biplab Sanyal, Olle Eriksson, Carla Puglia, and Barbara Brena — Department of Physics and Astronomy, Uppsala University, Sweden

Biphenylene ($C_{12}H_8$) is a promising candidate for applications in molecular electronics as well as a building block for two dimensional materials such as the biphenylene carbon (BPC) sheet, a possible alternative for graphene in nanoelectronics. The electronic structure of the gas phase biphenylene molecule is measured by core and valence level spectroscopy and detailed insights are revealed in conjunction with Density Functional Theory calculations. Hybrid functional calculations including the recently proposed OT-RSH functional are compared to GW calculations to provide an accurate theoretical description. Using the band structure obtained from GW calculations, we compute the optical adsorption spectrum by solving the Bethe-Salpeter equation of BPC. Typically for two-dimensional materials, a strong excitonic effect is found and bright and dark excitons are determined.

CPP 16.2 Tue 9:45 C 130

**Dimensionality of excitation transport in sol-gel-derived polymeric carbon nitride photocatalysts** — •Christoph Merschjann[1,2], Stefanie Tschierlei[1], Kamalakannan Kailasam[3], Arne Thomas[3], Dirk Hollmann[4], and Stefan Lochbrunner[1] — [1]Institut für Physik, Universität Rostock, D-18051 Rostock, Germany — [2]Freie Universität Berlin, D-14195 Berlin, Germany — [3]Leibniz-Institut für Katalyse, D-18059 Rostock, Germany — [4]Technische Universität Berlin, D-10623 Berlin, Germany

The spectral and temporal development of optically excited states in highly active sol-gel-derived polymeric carbon nitride (SG-CN) photocatalysts is investigated using time-resolved optical spectroscopy. By combining transient absorption results from a femtosecond pump-probe setup and transient photoluminescence using streak-camera investigations, the evolution of a light-emitting species appearing upon UV excitation is obtained. The emission decay reveals a universal power-law behaviour over more than seven decades in time (150 fs to 5 $\mu$s), the main difference between samples being the characteristic decay time in the nanosecond range. This finding is consistently described using a random-walk approach for the diffusive transport of light-induced polaron pairs, including both geminate and bimolecular recombination mechanisms. Thus, important features of the light-induced charge transport, namely the dimensionality and the regime of reasonable carrier mobilities, are deduced.

The validity of the approach is shown via comparison to ESR-based carrier-density measurements and photocatalytic activities.

CPP 16.3 Tue 10:00 C 130

**Simulation of Charge Transport in Organic Self-Assembled Monolayers for Applications in Field-Effect Transistors** — •Susanne Leitherer[1], Christof Jäger[2], Marcus Halik[3], Tim Clark[2], and Michael Thoss[1] — [1]Institute for Theoretical Physics, University Erlangen-Nürnberg, Germany — [2]Computer-Chemie-Centrum, University Erlangen-Nürnberg, Germany — [3]Institute of

Polymer Materials, University Erlangen-Nürnberg, Germany

We study charge transport through self-assembled monolayers (SAMs), which are used in field-effect transistors [1], employing a combination of molecular-dynamics simulations, semiempirical electronic structure calculations and Landauer transport theory. In particular, we investigate SAMs consisting of multifunctional molecules, where the active $\pi$-system is linked to a flexible insulating alkyl-chain. We find a close relation between the transport characteristics and the structural and electronic properties of the SAM [2]. For selected systems, we analyze pathways for efficient charge transport by examining local currents in the molecular layers. The pathways are compared to those obtained using Metropolis Monte Carlo (MC) path searches. In order to study the time-dependence of the preferred electron paths, we consider snapshots of the system selected at different times of a MD simulation. To further examine the influence of fluctuations on the transport properties, we utilize a time-dependent approach of charge transport using time-dependent nonequilibrium Green's function (NEGF) theory.

[1] C. Jäger *et al.*, J. Am. Chem. Soc. **135**, 4893 (2013)
[2] S. Leitherer *et al.*, J. Chem Phys. **140**, 204702 (2014)

CPP 16.4 Tue 10:15 C 130

**Quantum Molecular Dynamics Studies of Polymer-based Thermoelectric Materials** — •Håkan W. Hugosson, Amina Mirsakiyeva, and Anna Delin — Department of Materials och Nano Physics, Royal Institute of Technology KTH, Stockholm, Sweden

Using modern quantum molecular dynamics methods (QMD), where all the interactions are calculated from an electronic structure method (here density functional theory - DFT), we study the polymer-based thermoelectric material PEDOT and its charge carrying polarons. QMD simulations are parameter-free and enable a direct and potentially unbiased simulation of chemical and physical events. Since temperature is taken into account a sampling of the conformational space is made, also making simulations less biased upon choices of e.g. initial conditions and chosen reaction coordinates. Among these studies we will focus on the theoretical modeling of the properties and dynamics of polarons and bipolarons in PEDOT-oligomers and crystals and the effect of novel dopants in PEDOT.

Organic polymer-based thermoelectric materials (like PEDOT), unlike presently used inorganic thermoelectric materials composed of hazardous elements with low natural abundance, though presently being less efficient, can be mass-produced at a low cost using safer abundant elements.

CPP 16.5 Tue 10:30 C 130

**First-principles based descriptor for intrinsic charge carrier mobility in organic devices** — •Christoph Schober, Karsten Reuter, and Harald Oberhofer — Technische Universität München

In organic electronics charge carrier mobility is a key performance parameter. Due to the complex manufacturing processes of e.g. organic field effect transistors (OFETs) measured mobilities are often heavily affected by the device preparation. This masks the intrinsic materials properties and therewith hampers the decision whether further device optimization for a given organic molecule is worthwhile or not. Within hopping models based e.g. on Marcus theory the intrinsic mobility can be reliably calculated from first principles. Using a perturbative approach to this theory we formulate a descriptor that can be efficiently calculated for a wide range of organic molecules. For this descriptor we obtain good correlations to fully calculated mobilities, as well as to highest-quality experimental data where device preparation uncertainties are minimized. This suggests the descriptor as a useful tool for materials screening and quick assessment of device-related influences in measured mobilities.

CPP 16.6 Tue 10:45 C 130

**Effect of Mesoscale Ordering on the Energy Landscape of a Conjugated Polymer** — •Carl Poelking, Patrick Gemünden, Kurt Kremer, Kostas Daoulas, and Denis Andrienko — Max Planck Institute for Polymer Research, Mainz, Germany

A multiscale simulation approach is proposed to study the effect of morphology on charge transport properties of polymeric semiconductors, with poly(3-hexylthiophene) as a test case. The method incorporates both long-range conformational disorder and local ordering, and permits reintroduction of atomistic details into large-scale morphologies generated with a coarse-grained simulation approach. Based on the resulting atomistically resolved mesophases, we investigate how the energy landscape and spatial correlations thereof evolve with increasing degree of structural order in partially ordered systems. We show that a shift towards larger conjugation lengths plays a role in the amplification rather than formation of low-energy states, such that decreased energetic disorder rather than a decreased energetic mean characterize energetics in crystalline domains.

CPP 16.7 Tue 11:00 C 130

**The role of microstructure on charge transport in semicrystalline polymers** — •Riccardo Di Pietro[1], Iyad Nasrallah[2], Joshua Carpenter[3], Lisa Koelln[4], Lars Thomsen[5], Christopher R. McNeill[6], Antonio Facchetti[7], Harald W. Ade[3], Henning Sirringhaus[2], and Dieter Neher[4] — [1]Hitachi Cambridge Laboratory, UK — [2]University of Cambridge, UK — [3]North Carolina State University, Raleigh, USA — [4]University of Potsdam, Germany — [5]Australian Synchrotron, Clayton, Australia — [6]Monash University, Clayton, Australia — [7]Polyera Corporation, Skokie, USA

We present a study on charge transport on two widely used semiconducting polymers, P(NDI2OD-T2) and P3HT. Combining field effect transistor characterization and charge accumulation spectroscopy we provide a consistent and unambiguous correlation between the charge density dependence of mobility and the semicrystalline morphology of the polymer film. This new experimental evidence demonstrates that charge transport in semicrystalline polymers cannot be described using any currently available charge transport model such as multiple trap and release or variable range hopping. A new charge transport model is therefore proposed, which explicitly accounts for the presence of both crystalline and amorphous regions within the polymer film and for the coulobic repulsion between charge carriers accumulated within the same crystallite. It finally provides a coherent picture of charge transport that has important general consequences in regimes that are relevant not only for transistors but also diodes and solar cells.

**15 min. break.**

CPP 16.8 Tue 11:30 C 130

**The molecular structure of a high electron mobility n-type copolymer [P(NDI2OD-T2)] as studied by Infrared Transition Moment Orientational Analysis [IR-TMOA]** — •Arthur Markus Anton[1], Robert Steyrleuthner[2], Wilhelm Kossack[1], Dieter Neher[3], and Friedrich Kremer[1] — [1]Institut für Experimentelle Physik I, Universität Leipzig, Germany — [2]Fachberich Physik, Freie Universität Berlin, Germany — [3]Institut für Physik und Astronomie, Universität Potsdam, Germany

To investigate the molecular order in thin layers of P(NDI2OD-T2) a novel technique, named Infrared Transition Moment Orientational Analysis (IR-TMOA), is employed. Structure-specific vibrational bands are analyzed in dependence on *polarization and inclination* of the sample film with respect to the optical axis. Making use of IR specificity we deduce the molecular order parameter tensor for the respective moieties with regard to the sample coordinate system and determine separately the orientation of atomistic planes defined through the naphthalenediimide (NDI) and bithiophene (T2) units relative to the substrate, and hence, relative to each other. We observe that chlorobenzene causes the T2 planes to align preferentially parallel to the substrate at an angle of 29°. A chloronaphthalene:xylene mixture, instead, gives rise to a reorientation of the T2 units from a *face on* into an *edge on* arrangement (65 to 70°). In contrast, the NDI part remains basically unaffected. For both solvents, evidence for aggregated chains is observed by UV/vis absorption spectroscopy [Steyrleuthner et al., *J. Am. Chem. Soc.* **136** (2014)].

CPP 16.9 Tue 11:45 C 130

**Aerosol Jet-Printed Organic Thin Film Transistors - Performance Analysis and Optimization** — •Arno John, Hanna Krikcziokat, and Klaus Meerholz — Institut für Physikalische Chemie, Universität Köln

For the success of organic thin film transistors (OTFTs) in industrial applications it is essential to process devices by printing in order to radically lower production costs. Aerosol jet is a direct-write printing method which provides the user great control over material deposition. Along with layout flexibility and material compatibility, this makes this printing technology an excellent tool for fast prototyping devices.

We use aerosol jet technology to fabricate entire p- and n-type OTFTs by printing Ag-ink (source/drain electrodes), PTAA (p-type semiconductor) and N2200 (n-type semiconductor), PMMA (dielectric) and PEDOT:PSS (gate electrode). By varying parameters for individual components and evaluating the resulting transistors we optimize the printing process.

The performance of printed components is compared to evaporated and spin coated transistor components. We show that, with optimized processing parameters, it is possible to print transistors with charge carrier mobility, output current on/off ratio and threshold voltage of nearly equal quality of non-printed transistors.

CPP 16.10 Tue 12:00 C 130

**Investigation of semiconducting polymers with thermally cleavable side chains for application in multilayer devices I: Morphology and OFET devices.** — •Janusz Schinke[1,2], Sabina Hillebrandt[2,3], Milan Alt[2,5], Torben Adermann[2,4], Tobias Glaser[2,3], Annemarie Pucci[2,3], Norman Mechau[2,5], Manuel Hamburger[2,4], Wolfgang Kowalsky[1,2], and Robert Lovrincic[1,2] — [1]TU Braunschweig, IHF, Germany — [2]InnovationLab GmbH, Heidelberg, Germany — [3]U. Heidelberg, KIP, Germany — [4]U. Heidelberg, OCI, Germany — [5]KIT, Germany

Conjugated polymers enable the production of electronic devices from solution at room temperature due to their advantageous combination of their electrical, optical and film-forming properties. A major milestone for this emerging technology consists in achieving printed multi-layer functional devices. A great challenge for printed organic electronics is to deposit the subsequent layer of a multilayer component from the same solvent without destroying the underlying freshly deposited layer. The solubility reduction of semiconducting molecules by the external stimulus of heat is the aim of our work. Novel organic semiconductors bearing thermally cleavable side chains were investigated via AFM, ellipsometry, PE spectroscopy and IR spectroscopy. Their charge transport characteristics were studied using OFETs. These methods allow us to obtain a clear understanding of the pyrolysis process and its influence on the resulting performance. We achieve very homogeneous layers after thermal treatment which exhibit excellent solvent resistance and additionally show an increase in OFET performance.

CPP 16.11 Tue 12:15 C 130

**Following the evolution of nanomorphology in PEDOT:PSS electrodes in-situ** — •Claudia Palumbiny[1], Feng Liu[2], Thomas P. Russell[2], Alexander Hexemer[3], Cheng Wang[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]University of Massachusetts Amherst, Department of Polymer Science and Engineering, 120 Governors Drive, Amherst, MA 01003, USA — [3]Lawrence Berkeley National Lab, Advanced Light Source, 1 Cyclotron Road, Berkeley, CA 94720, USA

The strongest advantages of organic photovoltaics over classical semiconductors are the possibility of fully flexible devices and easy upscaling, e.g. by slot-die printing. For fully printed and flexible devices there is a strong need for non-brittle and solvent processed electrodes, such as highly conductive PEDOT:PSS. Film properties are strongly correlated to the films nanomorphology and with this strongly depend on the processing technique used. We investigate the film evolution of highly conductive PEDOT:PSS in-situ during the printing process. We monitor the film evolution by in-situ grazing incident wide angle scattering (GIWAXS). Five film formation processes are detected, the crystallization of the polymers is correlated to solvent evaporation and enhanced interchain coupling is induced by the use of high boiling point co-solvents as ethylene glycol. The enhanced conductivity in co-solvent treated PEDOT:PSS films is related to enhanced interchain coupling, change of the PEDOT to PSS ratio and crystallite sizes.

[1] Palumbiny et al., J. Phys. Chem. C 2014, 118, 13598.

CPP 16.12 Tue 12:30 C 130

**Angle resolved spectroscopy resolving local morphology of organic optoelectronic materials** — •Marius van den Berg, Anke Horneber, Kathrin Swider, Martin Meixner, and Dai Zhang — 1Institute of Physical and Theoretical Chemistry, University of Tübingen, Tübingen, Germany

The main component on which organic photovoltaic, transistor and photodetectors rely is the optoelectronic material. Knowledge about the local photophysical and photochemical properties of these materials at nanometer scale is important for improving overall performance and applicability [1]. The crystallinity and domain size of the local donor/acceptor morphology strongly affect the photon-electron conversion efficiencies of organic photovoltaics [2,3]. We aim at understanding the influences of nanometer scale morphology on the photophysical processes between donors and acceptors using a home built parabolic mirror assisted microscope. Using polarized excitation spectroscopy and angle resolved photoluminescence spectroscopy, we determine the relative degree of local structural order and molecular orientation in intact and photo degraded optoelectronic polymers. Furthermore, intensity changes in the angle resolved photoluminescence signals are compared with changes in the local photocurrent, to investigate morphology related photo degradation procedures, as well as the reversible/irreversible degradation steps in pi-conjugated polymers. 1)A. Dupuis et al. Eur. Phys. J. Appl. Phys. 56, 34104 (2011) 2)X. Wanget al. Small, 7, 2793 (2011) 3)R. Noriega et al. Nat. Mater., 12, 1038-1044, (2013)

CPP 16.13 Tue 12:45 C 130

**Multifunctional SNOM and its Application in Imaging Optoelectric Materials** — Anke Horneber, Marius van den Berg, Martin Meixner, Kathrin Swider, and •Dai Zhang — Institute of Physical and Theoretical Chemistry, University of Tübingen

Optoelectronic polymer material is the basic component in photovoltaic, photodetector, or transistor system. In organic photovoltaic, the photon-electron conversion efficiency is strongly influenced by the local donor/acceptor morphology, such as crystalline, or domain size.

To get insight into this topic, we developed multifunctional scanning near-field microscopy allowing simultaneously collecting correlated topographical, optical (Raman scattering and fluorescence), and photocurrent signals with nanometer scale resolutions [1-3]. The distributions and local morphology of donor or acceptor materials are imaged using the Raman fingerprints and scanning probe microscopes. The intensity ratios between the donor photoluminescence and the local photocurrent will be discussed, with respect to the charge transfer processes in films of different morphologies. Furthermore, photodegradation will be compared, especially in the aspects of local morphology, and optical properties. References: [1] Zhang, D. et al, Phys. Rev. Lett., 2010, 104, 056601. [2] Wang, X., Azimi, H., Zhang, D., et al, Small, 2011, 7, 2793. [3] Wang, X., Egelhaaf, H., Zhang, D., Adv. En. Mater, 2014, 1400497. [4] Wang, X., Broch K., Zhang, D. et al., J. Phys. Chem. Lett., 2014, 5, 1048.

## CPP 17: Microswimmers (joint session DY, BP, CPP)

Time: Tuesday 9:30–12:30 Location: BH-N 128

CPP 17.1 Tue 9:30 BH-N 128

**Trapping of active particles in inhomogeneous systems** — •Martin P. Magiera, Kevin Schröer, and Lothar Brendel — Fakultät für Physik, Universität Duisburg-Essen

Inhomogeneities in a system containing active particles can lead to an inhomogeneous particle distribution if they influence the particles' velocities [Schnitzer, PRE **48**, 2553]. Those may be caused, e.g., by inhomogeneous tumble rates of bacteria or inhomogeneous drive of men-made microswimmers [e.g. Buttinoni et al, PRL **110**, 238301].

Using Brownian dynamics simulations we show that such inhomogeneities can lead to particle accumulation in a prescribed passivity region where the activity of particles is suppressed, an effect interesting for applications. We derive a corresponding accumulation parameter with an extended Fick's law for inhomogeneous systems. Depending on the overall particle density a complete particle trapping can be observed. However, even if only a minority of particles is trapped, a tiny yield can act as a nucleation seed for larger agglomerates generated by dynamical clustering [Fily and Marchetti, PRL **108**, 235702] and pinned to the passivity region.

CPP 17.2 Tue 9:45 BH-N 128

**Statistics of passive tracers in an active fluid** — •Levke Ortlieb[1], Matthias Mussler[1], Christian Wagner[1], Thomas John[1], Philippe Peyla[2], and Salima Rafaï[2] — [1]Universität des Saarlandes — [2]Université Joseph Fourier - CNRS - LIPHY, Grenoble

In all aqueous suspension on earth there are various microswimmers, e.g. algae. In our experiments we tracked passive polystyrene particles with diameters from 1 to 3$\mu$m in suspension with the green alga Chlamydomonas reinhardtii at various concentrations. We used dark field microscopy for observations. The alga has a nearly spherical body of 5 to 10$\mu$m diameter and two flagella, which allow it to swims as a puller. We analysed the trajectories of the colloids statistically, in particular, the mean squared displacement and the probability density function (pdf) of position were computed. We found similarities to Brownian motion, as the mean squared displacement is proportional to time, but interestingly also a significant deviation was found: a non gaussian pdf of the tracer particle positions.

CPP 17.3 Tue 10:00 BH-N 128

**Characterization of Swimming Bacillus Subtilis** — •Javad Najafi[1], Thomas John[1], Gert Bange[2], and Christian Wagner[1] — [1]Experimental Physics, Saarland University, D-66123 Saarbruecken, Germany — [2]LOEWE Center for Synthetic Microbiology (Synmikro), Marburg, Germany

Bacteria can use flexible appendages called flagella to swim in aqueous environment. Our goal is to understand the influence of the number of flagella on the swimming behavior and efficiency. We study wild type strain of bacillus subtilis as a model system to unravel a few fundamental questions on swimming behavior of bacteria. Our microorganism is a peritrichous bacterium with about 25 flagella, and uses run and tumble strategy to explore its surrounding. Using dark field microscopy and tracking of single cell movements, we calculate statistics of swimming velocity, running and tumbling times, turning angles, diffusion coefficients and the temporal auto-correlations in changes of swimming directions. In further steps, we will investigate the influence of number of flagella on genetically engineered bacillus subtilus in aforementioned quantities.

CPP 17.4 Tue 10:15 BH-N 128

**Non-linear dynamics of self-organized ciliary beats** — •pablo sartori and frank julicher — Max Planck Institute for the Physics of Complex Systems. Noethnitzer Strasse 38 , 01187, Dresden, Germany.

The dynamic bending of cilia is driven by forces generated by dynein motor proteins. These forces slide adjacent microtubule doublets within the cilium. To create oscillatory beating patterns the activities of the dyneins must be coordinated both spatially and temporally. It is believed that this coordination occurs via the self-organization of the motors along the cilium, which are regulated by local strains such as sliding or cuvature. Yet which strain is the most relevant in regulation remains an elusive question.

In this work we show that self-organization of the motors is possible via a dynamic instability. We study the emerging beat patterns close and far from the critical point. By comparing two different motor regulatory mechanisms, sliding and curvature regulation, we conclude that the first only produces propulsion for long cilia, while the second does so also for short cilia. Our work thus suggests that short cilia may be regulated via curvature, and not sliding of the filaments.

CPP 17.5 Tue 10:30 BH-N 128

**Simulation of a microswimmer consisting of a four bead ring** — •Hendrik Ender and Jan Kierfeld — Lehrstuhl für Theoretische Physik I, Technische Universität Dortmund

Bead-spring structures undergoing cyclic shape changes in a viscous liquid can serve as model systems for artificial microswimmers. Closed ring-like bead-spring models can propel by cyclic shape changes, for example, induced by cyclic expansion and contraction of springs. Using multi-particle collision dynamics, we simulate a four-bead swimmer model in which the spheres are linked into a square-shaped ring structure. We show that cyclic changes of linker lengths give rise to a net swimming motion. The model can be generalized by including more beads into the ring structure and represents the first step towards the simulation of bigger ring or spherical swimmers, which propel by cyclic swelling and shrinking.

CPP 17.6 Tue 10:45 BH-N 128

**Spontaneous chiral symmetry breaking in model bacterial suspensions** — Rebekka E. Breier[1], Robin L. B. Selinger[2], Giovanni Ciccotti[3,4], Stephan Herminghaus[1], and •Marco G. Mazza[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Fassberg 17, 37077 Göttingen, Germany — [2]Chemical Physics Interdisciplinary Program, Liquid Crystal Institute, Kent State University, Kent, OH, USA — [3]Department of Physics, University of Rome "La Sapienza", P.le A. Moro 5, 00185 Rome, Italy — [4]School of Physics, University College Dublin, Belfield, Dublin 4, Ireland

Chiral symmetry breaking is ubiquitous in biological systems, from DNA to bacterial suspensions. A key unresolved problem is how chiral structures may spontaneously emerge from achiral interactions. We study a simple model of bacterial suspensions in three dimensions that effectively incorporates active motion and hydrodynamic interactions. We perform large-scale molecular dynamics simulations (up to $10^6$ particles) and describe stable (or long-lived metastable) collective states that exhibit chiral organization although the interactions are achiral. We elucidate under which conditions these chiral states will emerge and grow to large scales. We also study a related equilibrium model that clarifies the role of orientational fluctuations.

**15 min. break**

CPP 17.7 Tue 11:15 BH-N 128

**Velocity distributions in active Brownian suspensions** — •Zahra Mokhtari and Annette Zippelius — Institute for Theoretical Physics, Georg-August University of Goettingen

We study numerically a model of self-propelled polar disks in suspension. The active particles interact via hard-core elastic interactions and are driven along their axes, which are subject to rotational noise. We study the distribution of linear and rotational velocities, which are predicted to show strongly anomalous but largely universal features. We furthermore analyze the correlations due to the coupling of translational and rotational motion and show that the alignment of particles' velocities and orientations can be controlled by the damping.

CPP 17.8 Tue 11:30 BH-N 128

**Experimental setup for 3D tracking of artificial active microswimmers** — •Gunnar Klös, Carsten Krüger, Corinna C. Maass, and Stephan Herminghaus — Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany

During solubilisation in an aqueous surfactant solution well above the critical micelle solution, droplets of nematic liquid crystal show self-propelled swimming, driven by a Marangoni flow at the droplet interface [1]. These active pusher-type swimmers provide a potential physical model-system for micro-bioswimmers. We expect dimensional confinement to have a significant impact on their dynamics [2].

We have designed an experimental setup combining a microfluidic cell with a selective plane microscope using a scanning fluorescent light sheet [3]. At densities within the single scattering limit, trajectories of single swimmers or ensembles can be recorded under varying conditions of buoyancy, particle activity and cell geometry.

[1] S. Herminghaus et al., Soft Matter **10**, 7008 (2014). [2] E. Lauga et al., Biophys. J. **90**, 400 (2006). [3] J. Huisken et al., Science **305**, 1007 (2004).

CPP 17.9 Tue 11:45 BH-N 128

**Liquid crystal droplets as artificial microswimmers** — Carsten Krüger, Gunnar Klös, Chenyu Jin, Corinna C. Maass, •Christian Bahr, and Stephan Herminghaus — Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany

Droplets of common nematic mesogens show self-propelled motion (velocity up to 50 $\mu$m/s, typical droplet diameter 10 - 100 $\mu$m) when placed into aqueous phases containing ionic surfactants at concentrations considerably above the critical micelle concentration [1]. The self-propelled motion is fueled by the solubilization of the nematic droplet in the aqueous phase, resulting finally in the formation of a microemulsion in which all mesogenic molecules have been transferred from the initial droplet into the micelles of the ionic surfactant.

We report results concerning the dependence of the swimming behavior on various parameters (droplet size, surfactant concentration, etc.), the trajectories in different confinements, the collective behavior, and the influence of the nematic or isotropic state of the mesogenic droplets.

[1] S. Herminghaus, C. C. Maass, C. Krüger, S. Thutupalli, L. Goehring, and C. Bahr, Soft Matter **10**, 7008 (2014).

CPP 17.10 Tue 12:00 BH-N 128

**3D-tracking reveals how sperm find the egg** — Jan F. Jikeli[1], Luis Alvarez[1], •Benjamin M. Friedrich[2], and Laurence

Wilson[3] — [1]CAESAR, Bonn, Germany — [2]MPI PKS, Dresden, Germany — [3]University of York, York, UK

Sperm cells are guided to the egg by chemical cues in a process termed chemotaxis. We have previously put forward a theory of how sampling a concentration gradient along helical paths allows sperm of marine species to steer up-gradient [1]. Now, high-speed tracking in three space dimensions allows to probe sperm navigation live. We find that sperm display deterministic steering responses, which sets their chemotaxis strategy apart from those employed by most bacteria (biased random walk) or immune cells (spatial comparison). We dissect the control logic that links sensation and motor actuation in sperm chemotaxis. We find that control delays are close to their theoretical optimum for up-gradient navigation. The resultant navigation strategy is particularly well suited for fast swimmers operating at the limits of chemical detection. The choice of optimal navigation strategy of a search agent is tightly linked to its susceptibilities for noise [2].

[1] B.M. Friedrich *et al.*: Chemotaxis of sperm cells, *PNAS* **33**, 2007.
[2] L. Alvarez *et al.*: The computational sperm cell, *Trends in Cell Biology* **24**, 2014.

CPP 17.11 Tue 12:15 BH-N 128

**Complex lane formation in asystem of dipolar mircroswimmers** — •Florian Kogler and Sabine H. L. Klapp — Institute of Theoretical Physics, Secr. EW 7-1, Technical University Berlin, Hardenbergstrasse 36, D-10623 Berlin, Germany

We investigate the non-equilibrium structure formation of an experimentally motivated [1] two-dimensional (2D) binary system of dipolar colloids propelling in opposite directions. Using Brownian Dynamics simulations we find a transition towards a laned state, reminiscent of the laning transition in colloidal systems with isotropic repulsive inter actions. However, the strongly anisotropic dipolar interactions induce two novel features: First, lanes are characterized by a complex internal structure. Second, the laning transition displays reentrance with respect to the interaction strength. We interprete our findings by simple theoretical arguments relating the observed behaviour to general equilibrium properties of phase-separating fluids [2].

[1] S. Gangwal and O. J. Cayre and M. Z. Bazant and O. D. Velev, PRL 100 (2008) 058302.

[2] F. Kogler and S. H. L. Klapp, preprint

## CPP 18: On-Surface Polymerization (contributed session to SYOP, joint session CPP, MI)

Time: Tuesday 9:30–10:00 Location: C 243

CPP 18.1 Tue 9:30 C 243

**Covalent Coupling via Dehalogenation on Ni(111) supported Boron Nitride and Graphene** — •Claudius Morchutt[1,3], Jonas Björk[2], Rico Gutzler[3], and Klaus Kern[1,3] — [1]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]Department of Physics, Chemistry and Biology, IFM, Linköping University, 58183 Linköping, Sweden — [3]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Surface-assisted covalent coupling of organic molecules represents a bottom-up approach for growing defined 2D nanostructures which are promising candidates for a variety of potential applications such as membranes for gas storage/separation, active elements in (opto)electronic devices, and catalysis. Taking a step back from the standard synthesis on (coinage) metal surfaces we explored the polymerization of 1,3,5-tris(4-bromophenyl)benzene via dehalogenation on Ni(111) supported hexagonal boron nitride and graphene by scanning tunneling microscopy and density functional theory calculations. No polymerization is observed on bare Ni, whereas on h-BN/Ni(111) and graphene/Ni(111) molecules debrominate and couple into oligomers after annealing. DFT calculations reveal that both surfaces act as a heterogeneous catalyst and reduce the dehalogenation barrier significantly. They furthermore show a strong interaction between h-BN (graphene) and surface-stabilized radicals, which in turn explains the limited oligomer size as a consequence of a diffusion-limited process.

CPP 18.2 Tue 9:45 C 243

**Polymerization of polyelectrolyte poly-L-lysine on charge-patterned silicon wafers** — •Heidemarie Schmidt[1], Martin Müller[2], K. Wiesenhütter[3], B. Urban[2], A.-D. Müller[4], I. Skorupa[1,3], W. Skorupa[3], M. Rüb[5], and O.G. Schmidt[1,6] — [1]TU Chemnitz — [2]IPF Dresden — [3]HZDR — [4]Anfatec Instruments AG — [5]FH Jena — [6]IFW Dresden

The local modification of silicon surfaces by adsorbing polyelectrolytes has been predicted to become ubiquitous in the engineering of smart carriers for biosensors, tissue engineering, and directed cell growth [1]. We have implanted phosphorous ions in ca. 200-1000 nm thick layers of a silicon wafer, in order to realize a defined stripe-like microscopic pattern of surface-near electrostatic forces [2]. The estimated density of localized charges between the ca. 2-3 nm thick native silicon dioxide and the silicon wafer ranges from 10^14 to 10^18 m^-2 and is much larger and stable than charges from silanol groups at an ordinary silicon dioxide surface. Using combined Atomic and Kelvin probe force microscopy measurements we could show that cationic model polyelectrolyte poly-L-lysine (PLL) [3] with a single chain length of 200 nm is preferentially adsorbed in agglomerates with chain lengths of 1-2 micrometer on the implanted microsized regions of the silicon carrier at pH = 11. The unimplanted regions of the silicon wafer were comparatively weakly adsorbing the PLL. [1] H. Schmidt et al., Appl. Surf. Sci. 281 (2013) 24-29, [2] C. Baumgart et al., Phys. Rev. B. 80 (2009) 085305, [3] Advances in Polymer Science 255 & 256 (Ed.: Martin Müller), Springer, 2014

## CPP 19: Transport: Graphene (joint session TT, CPP, DS, DY, HL, MA, O)

Time: Tuesday 9:30–12:15 Location: A 053

CPP 19.1 Tue 9:30 A 053

**Observation of supercurrent in graphene-based Josephson junction** — •Libin Wang[1], Chuan Xu[2], Sen Li[1], Wencai Ren[2], and Ning Kang[1] — [1]Key Laboratory for the Physics and Chemistry of Nanodevices and Department of Electronics, Peking University, Beijing 100871, China — [2]Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China

Josephon junctions with a normal metal region sandwiched between two superconductors (S) are known as superconductor- normal-superconductor (SNS) structures. It has attracted significant attention especially when changing the normal metal with graphene, which allow for high tunability with the gate voltage and to study the proximity effect of the massless Dirac fermions. Here we report our work on graphene-based Josephon junction with a new two dimensional superconductor crystal, which grown directly on graphene, as superconducting electrodes. At low temperature, we observer proximity effect induced supercurrent flowing through the junction. The temperature and the magnetic field dependences of the critical current characteristics of the junction are also studied. The critical current exhibits a Fraunhofer-type diffraction pattern against magnetic field. Our experiments provided a new route of fabrication of graphene-based Josephon junction.

CPP 19.2 Tue 9:45 A 053

**Magnetoresistance of nanocrystalline and ion-irradiated graphene** — •Paul Linsmaier[1], Lorenz Weiss[1], Armin Shaukat[1], Christian Bäuml[1], Daniel Steininger[1], Ina Schneider[1], Matthias Büenfeld[2], Nils-Eike Weber[2], Andrey Turchanin[2], Miriam Grothe[3], Thomas Weimann[3], Ferdinand Kisslinger[4], Heiko B. Weber[4], and Christoph Strunk[1] — [1]Inst. f. Exp. and Appl. Physics, University of Regensburg — [2]Fac. of

Physics, University of Bielefeld — [3]Physikalisch-Technische Bundesanstalt, Braunschweig — [4]Fac. of Physics, F.-A. University Erlangen-Nürnberg

We investigate the magnetotransport in Hall bar structures of nanocrystalline graphene [1] compared to Ar$^+$-bombarded epitaxial graphene [2]. We measured the resistance $R(T)$ and $R(B)$ for samples with different sheet resistance (10-40 k$\Omega$/sq at $T = 300$K). The I-V characteristics of both types show strong non-linear behavior at low temperatures. Low resistive samples of nanocrystalline graphene show positive magnetoresistance (MR) with values up to + 60 % in perpendicular magnetic field for temperatures below a crossover temperature. Above this temperature the MR becomes negative. The perpendicular MR in the ion-bombarded graphene was always negative. In parallel magnetic field the MR exhibits large positive values up to + 700 % in the nanocrystalline graphene. Strongly non-monotonic behavior of the MR was observed in the ion-bombarded sample in parallel field.

[1] A. Turchanin et al., ACS Nano 5 (2011).
[2] K. V. Emtsev et al., Nat. Mat. 8, 203 - 207 (2009).

CPP 19.3 Tue 10:00 A 053

**Aharonov-Bohm effect in a graphene ring encapsulated in hexagonal boron nitride** — •Jan Dauber[1,2], Martin Oellers[1], Alexander Epping[1,2], Kenji Watanabe[3], Takashi Taniguchi[3], Fabian Hassler[4], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Aachen, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Jülich, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba, Japan — [4]JARA-Institute for Quantum Information at RWTH Aachen University, Aachen, Germany

Recent developments in the van der Waals assembly of heterostructures of two-dimensional materials enable the fabrication of graphene on substrate with very high quality. Outstanding charge carrier mobility and mean free path have been reported for micrometer sized samples of graphene encapsulated in hexagonal boron nitride (hBN). These unique electronic properties offer opportunities for the observation of rich mesoscopic transport phenomena in sub-micron sized graphene-hBN devices. Here, we present low-temperature magnetotransport measurements on a high mobility graphene ring encapsulated in hexagonal boron nitride. We observe the co-existence of weak localization, Aharonov-Bohm (AB) oscillations and universal conductance fluctuations. We investigate the periodicity of the AB oscillations as a function of charge carrier density and find clear evidence of the AB effect even at very low carrier densities. Finally, we report on the investigation of the AB oscillations in the cross over regime of emerging quantum Hall effect at reasonable magnetic fields.

CPP 19.4 Tue 10:15 A 053

**Ab-initio simulations of local current flows in functionalized graphene flakes and ribbons** — •Michael Walz[1], Jan Wilhelm[2], Alexei Bagrets[1], and Ferdinand Evers[3] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — [2]Institute of Physical Chemistry, University of Zürich, CH-8057 Zürich, Switzerland — [3]Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

Using our DFT-based transport framework AITRANSS [1], we calculate the transmission and the local current density in graphene flakes functionalized by adsorbed atoms, such as nitrogen or hydrogen. We find that even a single nitrogen atom can almost completely suppress the conductance of a (gated) graphene armchair nano-ribbon. In this situation local ring currents emerge that result in local (orbital) magnetic moments.

In addition, the current flow shows a highly inhomogeneous structure. In the absence of any scatters, the current flows along parallel streamlines that exhibit a strong lateral modulation [2]. In the presence of scattering centers, such as 20% hydrogen absorbants, we observe a filamentary pattern of streamlines. It exhibits local ring currents ("eddies") that go along with sizeable local magnetic fields, $\mathbf{B}(\mathbf{r})$. [3]

In the future, we plan to study the statistics of local currents of such large flakes and its dependency on the impurity concentration.

[1] A. Arnold, F. Weigend, F. Evers, J. Chem. Phys. 126 (2007)
[2] J. Wilhelm, M. Walz, F. Evers, Phys. Rev. B 89 (2014)
[3] M. Walz, J. Wilhelm, F. Evers, Phys. Rev. Lett. 113 (2014)

CPP 19.5 Tue 10:30 A 053

**Fabry-Pérot interference in monolayer and bilayer graphene devices** — •Ming-Hao Liu and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

Recent progress on high-quality graphene device fabrications has made submicron- or even micron-scale phase-coherent phenomena in graphene experimentally observable. Hence reliable quantum transport simulations for ballistic graphene devices are nowadays highly demanded. In this talk we give an overview on how such simulations can be accurately and efficiently performed. Concrete examples of Fabry-Pérot interference in single pn junctions in suspended monolayer graphene [1], multiple pn junctions in monolayer graphene on substrate [2], and pnp junctions in bilayer graphene encapsulated by hexagonal boron nitrite [3] will be briefly shown, as well as further studies of "electron optics" in graphene.

[1] P. Rickhaus, R. Maurand, M.-H. Liu, M. Weiss, K. Richter, and C. Schönenberger, Nature Comm. **4**, 2342 (2013);
M.-H. Liu, et. al., arXiv:1407.5620 (2014).
[2] M. Drienovsky, F.-X. Schrettenbrunner, A. Sandner, D. Weiss, J. Eroms, M.-H. Liu, F. Tkatschenko, and K. Richter, Phys. Rev. B **89**, 115421 (2014).
[3] A. Varlet, M.-H. Liu, V. Krueckl, D. Bischoff, P. Simonet, K. Watanabe, T. Taniguchi, K. Richter, K. Ensslin, and T. Ihn, Phys. Rev. Lett. **113**, 116601 (2014).

CPP 19.6 Tue 10:45 A 053

**Substrate-Induced doping of supported graphene: an ab initio study** — •Arezoo Dianat[1], Rafael Gutierrez[1], Zhongquan Liao[2], Martin Gall[2], Ehrenfried Zschech[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Fraunhofer Institute for Ceramic Technologies and Systems, D-01109 Dresden, Germany

A major challenge for applications of graphene in nanoelectronics is the absence of a band gap in its low energy spectrum. One possibility of gap opening is doping and there are various methods to achieve it: evaporation, thermal treatment, and plasma doping. In this study, using ab initio molecular dynamics, we investigate graphene doping mediated by substrate-induced mechanisms. More specifically, we address graphene on a B-doped Si(100) surface. Our ab initio total energy calculations show that B atoms prefer to locate on the surface layer of Si(100). Further, intercalation of B atoms into vacancy positions of graphene is only found for temperatures larger than 700 K. In a second step, the electrical transport properties of B-doped graphene are studied using the non-equilibrium Green's function approach.

**15 min. break.**

CPP 19.7 Tue 11:15 A 053

**Density of states of graphene with vacancies** — •Soumya Bera — MPI-PKS, Dresden

We numerically calculate the density of states (DOS) of graphene in the presence of compensated vacancy disorder. The model belongs to the BDI class of Atland-Zirnbauer symmetry classification of disordered metals, where the non-linear Sigma model predicts a Gade-type singularity in the DOS $\rho(E) \sim E^{-1}\exp(-|\log(E)|^{-1/2})$. We show that in the pre-asymptotic regime this is indeed true, however, at even lower energies the Gade-type behavior gives away to a stronger singularity of the form $\rho(E) \sim E^{-1}|\log(E)|^{-x}$ with $2 > x \geq 1$ in agreement with recent analytical work (Ostrovsky et al., PRL 113, 186803). We conclude that the generic Sigma model of the BDI class does not apply for strong (unitary) scatterers; the nature of disorder is of important to determine the low energy behaviour of disordered graphene.

[1] PRL 113, 186802 (2014).

CPP 19.8 Tue 11:30 A 053

**Nonlocal optical excitations and dynamic shear viscosity of graphene** — •Julia Link, Peter P. Orth, and Jörg Schmalian — Institute for Theoretical Condensed Matter physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe

We study the dynamic shear viscosity of the interacting electronic fluid of graphene in the finite frequency, collision-less regime, relevant for nonlocal optical properties. We determine the frequency dependence of the dynamic shear viscosity for non-interacting graphene and study the influence of the long-range Coulomb interaction. Finally we discuss a setup where the viscosity can be spectroscopically measured.

CPP 19.9 Tue 11:45 A 053

**Transport phenomena in deformed graphene: Magnetic field**

**versus curvature** — Thomas Stegmann[1,2] and •Nikodem Szpak[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany — [2]Instituto de Ciencias Fisicas, Universidad Nacional Autonoma de Mexico, Cuernavaca, Mexico

The current flow in deformed graphene nanoribbons is studied theoretically. Using a tight-binding model, we apply the nonequilibrium Green's function (NEGF) method to investigate how a localized deformation and a perpendicular magnetic field affect the current flow. At long wavelengths, the eikonal approximation applied to the effective Dirac equation leads to the Mathisson-Papapetrou equations describing trajectories of a spinning point-like particle in a curved space. We show that these trajectories are compatible with the current flow paths of the NEGF calculations. The deformation has two-fold effect on them: First, via a pseudo-magnetic field, with sixfold symmetry of attractive and repulsive regions, which acts differently on electrons and holes, but changes its sign when going from the K to the K' point. Second, via an attractive force due to the curvature of the ribbon, which treats electrons and holes equivalently. We conclude with an outlook on how to use deformed graphene ribbons for geometrical focusing of the current flow.

CPP 19.10 Tue 12:00 A 053

**Merging of the Dirac points in electronic artificial graphene** — •Juraj Feilhauer[1,2], Walter Apel[1], and Ludwig Schweitzer[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany — [2]Institute of Electrical Engineering, Slovak Academy of Sciences, Bratislava, Slovakia

Artificial graphene (AG) is a man-made electron system which has a similar bandstructure as normal graphene, i.e. in the low-energy part of the electronic spectrum, two bands touch and form a pair of Dirac cones. We study analytically and numerically the bandstructure of electronic AG under uniaxial strain. Here, AG is created from the two-dimensional electron gas by applying a repulsive triangular potential and the effect of strain is modeled by tuning the distance between the repulsive potentials along the armchair direction. In normal graphene, the theory based on nearest-neighbour tight-binding approximation predicts that due to the change of the hopping integrals by applying uniaxial strain, both Dirac cones are shifted away from the corners of the Brillouin zone and also becomes elliptical instead of circular. With increasing compressive strain, the Dirac cones move along the edge of Brillouin zone towards each other until they merge. We show that such a merging of the Dirac cones also exists in uniaxially compressed AG. With applied strain, we find the Dirac cones are also tilted and that can be simulated by the presence of a next-nearest-neighbour hopping in the tight-binding hamiltonian. We discuss a possible realization of our theoretical results in a recent experiment with molecular graphene.

## CPP 20: Membranes and vesicles I (joint session BP, CPP)

Time: Tuesday 9:30–12:30 Location: H 1028

**Invited Talk** CPP 20.1 Tue 9:30 H 1028

**Multifaceted BAR-domain proteins to shape cell membranes** — Coline Prévost[1], Mijo Simunovic[1,2], Henri-François Renard[1], Emma Evergren[3], Harvey McMahon[3], Ludger Johannes[1], Jacques Prost[1], Andrew Callan-Jones[4], and •Patricia Bassereau[1] — [1]Institut Curie, Paris, France — [2]University of Chicago, USA — [3]MRC, Cambridge, UK — [4]University Paris-Diderot, France

Cell plasma membranes are highly deformable and are strongly curved upon membrane trafficking or during cell motility. BAR-domain proteins with their intrinsically curved shape and their interaction with the actin cytoskeleton are involved in many of these processes.We have used in vitro experiments to study the interaction of BAR-domain proteins with curved membranes for understanding how inverted-BAR domain proteins such as IRSp53 are involved in the generation of filopodia and how the BAR-domain protein endophilin A2 can scission tubules induced by Shiga toxin internalization. We have pulled membrane nanotubes of controlled curvature from Giant Unilamellar Vesicles (GUVs) using optical tweezers and micropipette aspiration. With this approach coupled to theoretical modeling, we have evidenced for IRSp53 a protein phase separation along the nanotube occurring at low protein density for weakly curved membranes. It can explain the in vivo local clustering of the protein, a primary step in filopodia generation that precedes the recruitment of other partners. We have also shown that endophilin A2 scaffolds and stabilizes tubes in static conditions but induces scission when the tube is dynamically extended.

CPP 20.2 Tue 10:00 H 1028

**Measuring the composition-curvature coupling in binary lipid membranes by computer simulations** — •Israel Abraham Barragán Vidal and Marcus Müller — Institut für Theoretische Physik, Georg-August-Universität, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

This manuscript contributes to the field of biophysics, in particular, the formation of local composition inhomogeneities in model membranes (rafts). We present a simple phenomenological model to describe the effective coupling between curvature and composition in a two-component lipid bilayer. Beside the elastic contribution to the free energy and an intrinsic coupling between curvature and composition, our model also includes contributions from a composition- and curvature-dependent free energy of mixing.

Using an implicit-solvent model we extract the intrinsic composition-curvature coupling from computer simulations with planar and highly curved cylindrical bilayers. Beside the effective curvature-composition coupling, our computational strategy offers an alternative to obtain the spontaneous curvature from moments of the stress profile across a bilayer membrane. We expect this strategy will find further applications.

CPP 20.3 Tue 10:15 H 1028

**New Strategy to Study a Single SNARE Mediated Membrane Fusion Event** — •Jose Nabor Vargas[1], Kewin Howan[2], Andrea Gohlke[2,4], Ralf Seemann[1,3], Jean-Baptiste Fleury[1], and Frederic Pincet[2,4] — [1]Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Laboratoire de Physique Statistique, Ecole Normale Supérieure, 75005 Paris, France — [3]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [4]Department of Cell Biology, School of Medicine, Yale University, CT 06520 New Haven, USA

We present an approach to explore the properties of a single SNARE mediated membrane fusion event in a microfluidic chip. In a first step, a single free standing lipid membrane is generated at a defined position with the Droplet Interface Bilayer technique (DiB). In a second step, we inject a solution of divalent cations (Calcium, Ca2+) and small unilamellar vesicles functionalized with T-SNARE proteins (T-SUVs) around the planar membrane using a volume controlled flow. The presence of calcium mediates the direct fusion of the vesicles with the planar membrane, which is incorporating the proteins into the membrane. In a third step, we remove the calcium and the T-SUVs with a buffer solution. After this washing step, a solution of small unilamellar vesicles functionalized with V-SNARE proteins (V-SUVs) is injected around the planar membrane. And finally, we study single fusion event with good optical and electrical access.

CPP 20.4 Tue 10:30 H 1028

**Mechanics of the cell membrane coupled to the actomyosin cortex** — •Jochen A. M. Schneider and Guillaume Salbreux — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The cell membrane is the outer layer of a biological cell. It consists of lipids which form a two-dimensional fluid bilayer structure and is attached via linker proteins to the underlying actomyosin cortex, a thin network of actin filaments and myosin motors. In the past years, research has mainly focused on the physical description of the cell membrane and cytoskeleton independently. However, little is known on how they mechanically interact in the cell.

Here, we present a model for the interaction of membrane and cytoskeleton based on the assumption that the anchored membrane is attached to the underlying actomyosin cortex, subjected to active tension arising from myosin activity. Cell pressure results in membrane protrusions which can equilibrate their surface tensions by exchange of lipids. Using this physical description, we characterize how excess membrane area distributes around the cell. Based on a few fundamental cell parameters, the cortex tension, the membrane bending stiffness and the anchoring strength, we find a phase diagram with regions corresponding to a homogeneous distribution of membrane, to the pulling of membrane tubes and to the formation of one or several blebs. We finally use this result to discuss potential consequences for the mechanics of the cell.

CPP 20.5 Tue 10:45 H 1028

**Using Markov state models to obtain free energies of (de)mixing** — •Djurre H. de Jong and Andreas Heuer — University of Münster, Münster, Germany

Obtaining free energies of demixing in multicomponent systems, for example lipid bilayers, would greatly benefit many (theoretical) studies. For such systems the initial state, i.e. the mixed configuration, is often thermodynamically highly unstable. This can render standard techniques like umbrella sampling problematic.

We show that application of Markov state models to several short and independent simulations allows one to extract the free energy gain upon demixing very reliably. Here it is important that the temporal evolution of an appropriately defined order parameter displays local fluctuations. Specifically, this method is applied to a two component Ising model and a binary Lennard-Jones system.

**15 min break**

CPP 20.6 Tue 11:15 H 1028

**The Mechanism of Phagocytosis: Two Stages of Engulfment** — •David M. Richards and Robert G. Endres — Imperial College London, UK

Despite being of vital importance to the immune system, the mechanism by which cells engulf relatively large solid particles during phagocytosis is still poorly understood. From movies of neutrophil phagocytosis of polystyrene beads, we measure the fractional engulfment as a function of time and demonstrate that phagocytosis occurs in two distinct stages. During the first stage, engulfment is relatively slow and progressively slows down as phagocytosis proceeds. However, at approximately half-engulfment, the rate of engulfment increases dramatically, with complete engulfment attained soon afterwards. By studying simple mathematical models of phagocytosis, we suggest that the first stage is due to a passive mechanism, determined by receptor diffusion and capture, whereas the second stage is more actively controlled, perhaps with receptors being driven towards the site of engulfment. We then consider a more advanced model that includes signalling and captures both stages of engulfment. This model predicts that there is an optimum ligand density for quick engulfment. Further, we show how this model explains why non-spherical particles engulf quickest when presented tip-first.

CPP 20.7 Tue 11:30 H 1028

**No spatial spreading of chemotactic signaling in amoeboid cells upon receptor stimulation** — •Matthias Gerhardt, Michael Walz, and Carsten Beta — Institut für Physik und Astronomie, Karl-Liebknecht-Strasse 24/25, 14476 Potsdam, Germany

Recently we have shown that in chemotactic Dictyostelium discoideum cells stimulation of a confined membrane region with cAMP leads to confined signaling of PIP3, PTEN, and filamentous actin. A consequence of this observation is that cAMP stimuli cannot trigger spatial spreading of intracellular signaling. However, in the absence of an extracellular cAMP stimulus, components of the signal transduction system where observed to form traveling waves that show all hallmarks of an excitable system. This excitable system is characterized by PIP3-rich membrane regions circumscribed by actin segments propagating together as a composite wave across the substrate attached membrane of a Dictyostelium cell. Since cAMP stimulation causes depletion of such waves, we concluded there must be an intracellular switch, which determines whether the signal transduction is excitable or not. Since earlier observations show that a [betagamma]G knockout remarkably enhances PI3K activity, we conjecture that the PI3K is a suitable candidate to take on the role of an intracellular switch which controls excitability.

CPP 20.8 Tue 11:45 H 1028

**Recognition Force Spectroscopy on Lamellar Body Surfactants collected from Primary Alveolar Cells Type II** — •Patrick Paul[1], Nina Hobi[2,3], Susanne Rappl[1], Thomas Haller[3], Manfred Frick[2], and Kay E. Gottschalk[1] — [1]Institute of Experimental Physics, Ulm University, Ulm, Germany — [2]Institute of General Physiology, Ulm University, Ulm, Germany — [3]Department of Physiology and Medical Physics, Division of Respiratory Cell Physiology, Medical University of Innsbruck, Innsbruck, Austria

Type II pneumocytes produce and secrete pulmonary surfactant into the alveoli of the lung. Surfactants lower the surface tension between the air-liquid interface within the alveoli. Surfactant consists of multilayers of lipids, mainly phosphatidylcholine, and specific, embedded surfactant proteins (SP-B and SP-C). Physiological studies demonstrated that these proteins play a major role in the stability of the surfactant [1]. However, the precise nature and exact structure of how these proteins are arranged within the lipids is yet unknown.

Hence, we imaged the structure of SP-B and SP-C assembly within a single-lipidlayer surfactant with single molecule force spectroscopy.

Reference: [1] Jesús Pérez-Gil, Structure of pulmonary surfactant membranes and films: The role of proteins and lipid-protein interactions, 2008, Biochimica et Biophysica Acta 1778, 1676-1695

CPP 20.9 Tue 12:00 H 1028

**Local viscosities near plasma membranes of living cells** — •Felix Jünger and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, University of Freiburg, Georges-Koehler-Allee 102, 79110 Freiburg, Germany

The molecular processes of particle binding and endocytosis are influenced by the locally changing mobility of the particle nearby the plasma membrane of a living cell. Close to different cellular interfaces, the viscous drag $\gamma$ changes strongly with the distance to the interface. In our work we use photonic force microscopy (PFM) to investigate how $\gamma$ changes when an optically trapped $1\mu$m polystyrene bead approaches the plasma membrane of different biological cells. The bead's temporal fluctuations are tracked interferometrically in three dimensions with nanometer precision and on a microsecond time scale. The autocorrelation of the bead's motion reveals the friction coefficient $\gamma$(d) as a function of bead-membrane distance d. We find a simple exponential decay for $\gamma$(d) with a hydrodynamic decay length $\Lambda$(d) that fits well to the obtained experimental data. We investigated different cell types (J774, HT29, MDCK) and a giant unilamellar vesicle (GUV). We find that all values $\Lambda$(d) measured at biological membranes are significantly longer than those of a rigid glass coverslip, giving rise to the conclusion that the deformable shape of the membrane influences the hydrodynamic interaction.

CPP 20.10 Tue 12:15 H 1028

**Fluorescence Imaging of Light Induced Reactive Oxygen Species (ROS) in Plant Cell Tissue** — •Franz-Josef Schmitt[1], Vladimir Kreslavski[2], Galina N. Schirshikova[2], Csongor Keuer[1], Sergei K. Zharmukhamedov[2], Suleyman I. Allakhverdiev[2], and Thomas Friedrich[1] — [1]Institute of Chemistry, Bioenergetics, TU Berlin, Berlin, Germany — [2]Institute of Basic Biological Problems, RAS, Pushchino, Moscow Region, Russia

UV-radiation in combination with toxic compounds like polyaromatic hydrocarbons (PAHs) lead to generation and accumulation of reactive oxygen species (ROS) in animal and plant cells. ROS generation by naphthalene (Naph), a lipophilic PAH, was studied with fluorescence microscopy employing the ROS sensitive dye dichlorofluorescein (DCF). Under high light illumination, Naph-treated leaves of Arabidopsis thaliana showed the spread of ROS waves across the tissue with a period time of 20 min. The reduction of PSII activity at the presence of Naph was accompanied by transient generation of hydrogen peroxide as well as swelling of thylakoids and distortion of cell plasma membranes. It could be shown that Naph treated leaves of Arabidopsis thaliana show enhanced DCF fluorescence in the thylakoid membrane. The comparison of short term and long term exposure to different PAHs revealed that at short term exposure, the PAHs with high water solubility lead to the strongest reduction of PS II activity while after long term exposure the effect of PAHs with low water solubility is stronger.

# CPP 21: Polymer dynamics

Time: Tuesday 9:30–13:00 Location: C 264

CPP 21.1 Tue 9:30 C 264

**Self-Entanglement of a Long Polymer Chain** — •Diddo Diddens, Albert Johner, and Jörg Baschnagel — Institut Charles Sadron, Université de Strasbourg, 23 Rue du Loess, BP 84047, 67034 Strasbourg Cedex 2

We study the effective interaction between the two halves of a long polymer chain under Θ-conditions by both Monte Carlo and Molecular Dynamics simulations. It is well known that in good (poor) solvents, different chain segments repulse (attract) each other, whereas these two opposing effects roughly cancel in the vicinity of the Θ-point. However, the *topological* self-interaction of long polymer chains under these conditions is less clear, which motivated our present analysis.

In a first step, we analyze structural properties such as the number of monomeric contacts between the two halves of the chain as well as characteristic topological quantities. Subsequently, we focus on the dynamical processes leading to the disengagement of the two halves after cutting the chain in the middle. This question is relevant for stimuli-responsive materials, in which e. g. the central bond of a long polymer chain is cleaved photochemically. Another motivation stems from biological issues such as the enzymatic cutting of long DNA/RNA strands in a crowded medium, which also involves the disengagement of distinct parts of long polymer chains. Finally, we will give a brief account on other architectures such as polymer stars.

CPP 21.2 Tue 9:45 C 264

**Numerical rate theory approach to polymer escape** — •Harri Mökkönen[1,2], Tapio Ala-Nissila[1], and Hannes Jónsson[1,2] — [1]Department of Applied Physics and COMP CoE, Aalto University School of Science, P.O. Box 1100, FIN-00076 Aalto, Espoo, Finland — [2]Faculty of Physical Sciences, University of Iceland, Reykjavik, Iceland

The polymer escape problem in an external double well potential is studied. The polymer is known to cross the energy barrier in a coiled form below critical length $N_C$ and in a stretched form above $N_C$, corresponding to so called "kink" solution in instanton theory [1,2]. We perform Brownian dynamics simulations to obtain the crossing rate $\mathcal{R}_{\mathrm{MD}}$ as a function of the chain length $N$ and the spring constant $K$. We numerically find the minimum energy path of the transition and by using the harmonic approximation of transition state theory recover the crossing rate $\mathcal{R}_{\mathrm{HTST}}$ agreeing with the simulations up to $N_C$. Above $N_C$ the energy barrier of the transition becomes flat so the crossing rate by harmonic approximation fails to give the quantitatively correct rate. We study the diffusive mechanism on top of the flat barrier to obtain dynamical corrections $f(N)$ for the harmonic approximation of the crossing rate $\mathcal{R}' = f(N)\mathcal{R}_{\mathrm{HTST}}$.

[1] S. K. Lee and W. Sung, *Phys. Rev. E* **63**, 021115 (2001).

[2] H. Mökkönen, T. Ikonen, H. Jonssón, T. Ala-Nissila, *J. Chem. Phys.* **140**, 054907 (2014).

CPP 21.3 Tue 10:00 C 264

**Dynamics of Living Polymers** — •Ali Malek. and Reiner Kree — Georg August Universität Göttingen

Living polymers constitute an important class of active soft matter. They refer to a large class of polymers whose lengths are ever changing. These changes in length, in many cases, is due to addition (polymerization) or subtraction (depolymerization) of monomer units at their active ends. We construct an analytically tractable model for a flexible chain (Rouse Model), which grows in length by a power law $l(t) = \gamma t^{\alpha}$. We find asymptotically exact solutions in the long-time regime, which allow to calculate the dynamical structure and the rheological properties both for free and forced chains. Our analytical results agree with simulations for times larger than a crossover time $t_c$. As a result we give new scaling laws for end-to-end distance correlation, the viscosity and the force against a wall.

CPP 21.4 Tue 10:15 C 264

**Studying linear and nonlinear viscoelasticity of highly entangled polymer melts with computer simulations** — •Guojie Zhang, Torsten Stuehn, Kostas Daoulas, and Kurt Kremer — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128, Mainz, Germany

Viscoelasticity of entangled polymeric liquids is important for both basic science and industrial applications, e.g. polymer processing. Particularly important is the regime of nonlinear viscoelastic behavior, which however is still not well understood. Using computer simulations, we focus on obtaining a molecular understanding of chain retraction process in entangled polymers under a large step-strain. Benefiting from a simulation scheme recently developed, equilibrated configurations of high molecular weight polymer melts (number of entanglements per chain Z > 100) described with microscopic details are generated. Regimes of linear and nonlinear viscoelasticity of entangled polymers are addressed by imposing a stepwise strain on these samples. In those highly entangled melts, a clear plateau modulus is observed in the linear regime (e.g. small step strain). A quantitative agreement between value of entanglement length estimated from the plateau modulus and that measured from primitive path analysis is found. To study chain retraction process in nonlinear regime, we monitor the evolution of entanglement densities and single-chain structure factor in a largely strained sample.

CPP 21.5 Tue 10:30 C 264

**Relaxation of Semiflexible Polymers with Branching, Loops, and Dihedral Interactions** — •Maxim Dolgushev — Theoretical Polymer Physics, University of Freiburg, Germany

This talk concentrates on recent advances in the mathematical-analytical theory of semiflexible polymers[1-3]. Based on the framework of semiflexible treelike polymers[4] as well as on its further extensions, the following results of new investigations will be presented:

(1) The study of the orientational relaxation of the single segments in semiflexible dendrimers [1]. Here, focusing on the NMR relaxation functions, it has been shown that including bending rigidity allows one to distinguish between segments for different dendrimer's shells, whereas the fully flexible model does not show such a feature.

(2) The basic model of Ref. [4] involves only angular restrictions. A next step forward is devoted to the investigation of the role of dihedral constraints. Remarkably, also in this, more complex situation one can obtain analytic results, as we show for linear chains [2].

(3) The semiflexibility constraints are introduced in a mean-field way [2,4], i.e. they do not reduce the number of degrees of freedom. However, for polymers with loops the closure conditions represent strict holonomic constraints. These can be taken into account based on the penalty function method [3].

[1] D.A. Markelov et al., J. Chem. Phys. 140, 244904 (2014).

[2] M. Dolgushev, A. Blumen, J. Chem. Phys. 138, 204902 (2013).

[3] M. Dolgushev et al., J. Chem. Phys. 141, 014901 (2014).

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

CPP 21.6 Tue 10:45 C 264

**Entropic segregation of ring polymers confined to a cylinder** — •Elena Minina and Axel Arnold — Institute for Computational Physics, University of Stuttgart, Allmandring 3, 70569, Stuttgart, Germany

Newly replicated circular chromosomes segregate inevitably during cell division in elongated primitive bacteria such as E.coli. Although many proteins surrounding the chromosomes are possibly involved in this process, the chromosomes would also move apart without these. The reason is, that overlapping chromosomes lose conformational entropy, and the only chance to gain this entropy is to segregate. In the present study we investigate entropic segregation of ring polymers confined to a cylinder. Using MD simulations and renormalized Flory theory, we estimate how fast overlapping rings segregate and show that the obtained results can be explained by previous results on linear polymers and a simple rescaling argument. This rescaling is based on an argument that a ring can be treated as two independent chains trapped in smaller subcylinders. Our results indicate that this argument can be extended to arbitrary amounts of overlapping chains occupying different amounts of space. The polymers however start segregation only after the initial symmetry of full overlap has been broken. This induction happens by rearranging the polymer ends. We previously showed for linear chains, that this induction time grows exponentially with the polymer length, making segregation a rather slow process. The ring topology however facilitates the segregation process reducing the induction time significantly compared to linear polymers.

CPP 21.7 Tue 11:00 C 264

**Chain Dynamics near the Unentangled-Entangled Transi-**

**tion** — •Herwin Jerome Unidad[1], Michaela Zamponi[1], Oxana Ivanova[1], Lutz Willner[2], Wim Pyckhout-Hintzen[2], Andreas Wischnewski[2], Dieter Richter[1,2], and Lewis Fetters[3] — [1]JCNS, Outstation at MLZ, Forschungszentrum Juelich, Garching, Germany — [2]JJCNS-1/ICS-1, Forschungszentrum Juelich, Juelich, Germany — [3]Department of Chemical and Biological Engineering, Cornell University, Ithaca, New York

It is well-known that the transition between unentangled to entangled dynamics occurs at a critical molecular weight (Mc), typically assumed to be twice the entanglement molecular weight (Me). Recently, we have reiterated a previous finding that the ratio between Mc and Me doesn't assume a universal value of 2 for all polymer melts but in fact shows a dependence on the packing length (p). Not withstanding, the physical picture behind the independent existence of Me and Mc remains unclear.

Here, we reinvestigate the problem by probing the microscopic dynamics of polybutadiene melts near the transition by neutron spin echo spectroscopy. We analyze the dynamic structure factor within the framework of the Rouse model with modified mode spectrum. We find that suppression of long-wavelength modes in the spectra already occurs for melts with molecular weight above Me, even if they are still below Mc. We rationalize these results based on earlier ideas on entanglement formation. We also apply this framework in confronting our viscosity data for various polymers.

**15 min. break.**

CPP 21.8 Tue 11:30 C 264

**Model-free information on polymer dynamics from neutron backscattering** — •Felix Roosen-Runge and Tilo Seydel — Institut Laue-Langevin, Grenoble, France

Quasi-elastic and inelastic neutron backscattering is well-suited to study dynamics at time scales of several pico- to nanoseconds and nanometer length scales. Dynamical transitions in polymers versus temperature or time can been monitored via the mean-squared displacement obtained in a model-free way from scans of the elastic scattering at zero neutron energy transfer. Recent instrument updates at the spectrometer IN16B (Institut Laue-Langevin, Grenoble) allow for so-called inelastic fixed window scans (IFWS) at fixed non-zero neutron energy transfer [1]. In combination with the achieved high flux, IFWS allow to monitor dynamics in more detail, e.g. focusing on tunnel spectra. A generalized mean-squared displacement from IFWS can be used as a model-free indicator of confined and anomalous diffusion [2]. We outline the power of the IFWS using analytical results for the measured quantities. Our results allow a direct evaluation of the effect of instrumental resolution on the measured mean-squared displacement. We discuss further application of IFWS such as monitoring dynamical heterogeneities in the sample.

[1] B. Frick et al., Nucl. Instrum. Meth. A 669, 7 (2012)

[2] F. Roosen-Runge, T. Seydel, EPJ Web of Conferences, in press

CPP 21.9 Tue 11:45 C 264

**Shear-induced ordering or disentaglement?** — •Ulrich Scheler — Leibniz-Institut für Polymerforschung Dresden e.V.

Rheo NMR permits the investigation of molecular dynamics in a wide range of correlation times of polymer melts or solutions under shear in a Couette cell. transverse relaxation T2 is strongly affected by the slow dynamics of polymer chain segments. One would expect a strong shortening of T2 as a result of shear-induced ordering of the polymer chains in a Couette cell. However the opposite is observed T2 becomes longer in melts of poly(propylene) and solutions of poly(styrene sulfonate), which can be explained by a loss of entanglements as a result of the shear.

CPP 21.10 Tue 12:00 C 264

**Bottlebrush melts** — •Jaroslaw Paturej[1,2], Sergei Sheiko[3], and Michael Rubinstein[3] — [1]Leibniz-Institut of Polymer Research, Dresden, Germany — [2]Institute of Physics, University of Szczecin, Szczecin, Poland — [3]Department of Chemistry, University of North Carolina, Chapel Hil, NC, USA

A bottlebrush polymer is a branched macromolecule composed of a linear chain (backbone) with sidechains densely tethered to it. High grafting density of side chains gives rise to various unique structural properties, such as highly extended conformations of their backbones and tunable character of their stiffness and rheological properties with degree of polymerization of the side chains. We conducted coarse-grained molecular dynamics simulations to determine how the number of Kuhn segments in a bottlebrush backbone $L$ and in the sidechains $N$ affect size, stiffness, and structure of these molecules. We found that the size (mean-squared radius of gyration and end-to-end distance) and persistence length of bottlebrushes in a melt state scales as $N^{1/2}$.

CPP 21.11 Tue 12:15 C 264

**Thermophoresis of linear polymers: is it Rouse or Zimm?** — •Werner Köhler[1] and Konstantin Morozov[2] — [1]Physikalisches Institut, Universität Bayreuth, D-95440 Bayreuth, Germany — [2]Department of Chemical Engineering, Technion Israel Institute of Technology, Haifa 32000, Israel

Polymer thermophoresis, the migration of dissolved polymer chains along a temperature gradient, is independent of molar mass for sufficiently long chains. Systematic experiments in our group have shown that the relevant units are not the monomers but rather correlated entities of the size of the Kuhn segment. The molar mass independent thermophoretic mobility has been interpreted in the literature in terms of a Rouse-type dynamics based on a draining coil model. Recent results reported for linear chains, crosslinked microgels, and core-shell particles of the thermoresponsive polymer PNIPAM together with older data for copolymers suggest, however, a non-draining coil with hydrodynamic coupling (Zimm). We show that the relevant thermophoretic interactions decay $\propto r^{-2}$ and, thus, much slower than the short-ranged ($\propto r^{-6}$) van der Waals interactions. In consequence, thermophoresis results from volume rather than surface forces. The hydrodynamic flow penetrates only into a boundary layer of the coil and causes tangential stress on the coil as a whole, and not on the scale of the individual segments. The experimentally observed molar mass independence of the thermophoretic mobility naturally follows from the model.

CPP 21.12 Tue 12:30 C 264

**Water enhanced dynamics of cellulose paper** — •Björn Kuttich, Ann-Kathrin Grefe, and Bernd Stühn — Experimental Condensed Matter Physics, TU Darmstadt, Germany

With over 50 weight percent cellulose represents the main part of plant cells. In terms of soft matter physics it is a rather complex and important biopolymer. Corresponding to its biological application cellulose is insoluble in water, but due to the monomers hydroxy groups it has a hygroscopic tendency. In industrial applications cellulose is the major component of paper, where water uptake can become important during manufacturing or processing.

While hydration effects on crystalline cellulose are already investigated the dynamics in cellulose papers, where highly oriented cellulose fibres are used, are less understood. In this work we therefore focus on a systematic variation of the hydration level of cellulose paper with different porosities. By using a hydration chamber for the humidification process, in which the relative air humidity can precisely be tuned, a water content in the sample between a few weight percent of water up to almost 20 percent can be realised. While our investigations by dielectric spectroscopy show only minor influences of the papers porosity, accelerated dynamics due to the presence of water become apparent. In contrast to the acceleration also the suppression of a local relaxation mode, which is not observed for crystalline cellulose, is found. To monitor water uptake of the sample and its characteristic time scale, all measurements are accompanied by time resolved weighing experiments, which reveal an uniform hydration process.

CPP 21.13 Tue 12:45 C 264

**Glassy dynamics of Poly(2-Vinyl-Pyridine) brushes with varying grafting density** — •Nils Neubauer[1], René Winkler[2], Martin Tress[1], Petra Uhlmann[2], Manfred Reiche[3], and Friedrich Kremer[1] — [1]Molecular Physics, Institute of Experimental Physics I, Leipzig University, 04103 Leipzig, Germany — [2]Nanostructured Materials, Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany — [3]Experimental Department II, Max Planck Institute of Microstructure Physics, 06120 Halle (Saale), Germany

The molecular dynamics of poly(2-vinyl-pyridine)(P2VP) brushes is measured by Broadband Dielectric Spectroscopy (BDS) in a wide temperature ($250\,\mathrm{K} - 440\,\mathrm{K}$) and broad spectral ($0.1\,\mathrm{Hz} - 1\,\mathrm{MHz}$) range. This is realized using nanostructured highly conductive silicon electrodes being separated by silica spacers as small as $35\,\mathrm{nm}$. A "grafting-to"-method is applied to prepare the P2VP-brushes with five different grafting densities ($0.03\,\mathrm{nm}^{-2} - 0.12\,\mathrm{nm}^{-2}$), covering the "true-brush" regime with highly stretched coils and the mushroom-to-brush transition regime. The film thickness ranges between 1.8 to 7.1 ($\pm$ 0.2) nm. Two relaxations are observed, an Arrhenius-like process being attributed to fluctuations in the poly(glycidyl methacrylate) (PGMA) linker used for the grafting reaction and the segmental dynamics (dynamic glass transition) of the P2VP brushes. The latter is characterized by a Vogel-Fulcher-Tammann dependence similar to bulk P2VP. The results can be comprehended considering the length scale on which the dynamic glass transition ($\leq$ 1 nm) takes place.

# CPP 22: Charged Soft Matter I

Time: Tuesday 9:30–11:30 Location: PC 203

CPP 22.1 Tue 9:30 PC 203

**Dielectric properties of ionic liquids** — •Grigory Zarubin and Markus Bier — Max Planck Institute IS and University of Stuttgart, Germany

The study of the dielectric properties of room temperature ionic liquids (RTILs) is an important task since RTILs are used as solvents in chemical reactions and the knowledge of their global solvation capability is crucial. Moreover, investigation of the dielectric properties, e.g. via the dielectric function $\varepsilon(k)$, does not require sophisticated computer simulations on the atomistic level because one is concerned with the behavior of the system on large length scales. Thus, a coarse grained model of a dense fluid of charged hard spheres (restricted primitive model, RPM) is assumed to be sufficient. The dielectric properties of the ionic liquid model were investigated with the help of Monte Carlo (MC) simulations. The electrical susceptibility $\chi(k) = \varepsilon(k) - 1$ has been calculated and it was assumed to have two constituents: i) $\chi_{ind}(k)$ corresponding to the induced charge polarization and ii) $\chi_{orient}$ corresponding to the orientation of effective dipoles formed by neighboring cation-anion pairs. The comparison of $\chi_{ind}$ and $\chi_{orient}$ showed that the ionic liquid is equivalent to a purely dipolar fluid for external static nonuniform electric fields of wavelengths $\lambda \leq \sigma$ with $\sigma$ being the diameter of the cation (anion). An attempt to describe the orientational component $\chi_{orient}$ analytically in the framework of density functional theory (DFT) has been made. DFT within modified mean-field approximation is able to describe the computer simulation results quantitatively in the longwavelength limit ($k \to 0$).

CPP 22.2 Tue 9:45 PC 203

**Thermal and structural properties of dense ionic liquids** — •Hendrik Bartsch and Markus Bier — Max Planck Institute IS and University of Stuttgart, Germany

The phase behavior and the structure of ionic liquids has been a subject of many theoretical studies, simulations and experiments. However, it has not been investigated so far which features of the underlying Coulomb interaction lead to the properties of ionic liquids. The aim of this work is to answer the fundamental question, whether the long-range character or the valency dependence of the Coulomb interaction determine the thermal and structural properties. In order to investigate the influence of the interaction range a modified Lattice Restricted Primitive Model is considered, where the electrostatic interactions are truncated at finite distance. Structural and thermal properties are obtained via grandcanonical Monte Carlo simulations as functions of the cut-off radius. The critical temperature of the modified LRPM is found to be an order of magnitude too high as compared to the ordinary LRPM of the long-ranged Coulomb interaction. Additionally, we observe a strong dependence of the critical temperature on the cut-off radius which does not appear to converge towards the correct value in the long-range limit. We show by means of an appropriately improved model that this defect does not occur and that the quantitatively correct phase behavior and structure can be obtained if charge neutrality within the interaction range, which corresponds to the perfect screening property, is maintained.

CPP 22.3 Tue 10:00 PC 203

**Solvent effects of 1-Ethyl-3-methylimidazolium acetate** — •Volker Lesch[1], Andreas Heuer[1], Christian Holm[2], and Jens Smiatek[2] — [1]Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster — [2]Institut für Computerphysik, Universität Stuttgart

Room temperature ionic liquids (RTILs) are promising candidates for several applications due to their properties with regard to thermal stability and ionic dissociation. For example the usage as electrolytes or solvents is investigated. Furthermore, they are less hazardous compared to other solvents.

In this study, we focus on solvation effects of 1-ethyl-3-methylimidazolium acetate. Therefore, we conducted molecular dynamics simulations of this ionic liquid combined with uncharged and charged spheres. We investigated the solvation behavior and the dynamics of the spheres. We found perturbation in the ordering of the ionic liquids also for long distances, even for the neutral sphere. The reason for this perturbation are electrostatic interactions.

CPP 22.4 Tue 10:15 PC 203

**A joint theoretical/experimental study of lithium ion dynamics in ionic liquids/lithium salt mixtures** — •Volker Lesch[1], Sebastian Jeremias[2], Sangsik Jeong[3,4], Yudong Zhan[3,4], Arianna Moretti[3,4], Stefano Passerini[3,4], Oleg Borodin[5], and Andreas Heuer[1] — [1]Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster — [2]MEET, Universität Münster — [3]Helmholtz Institute Ulm — [4]Karlsruhe Institute of Technology — [5]U. S. Army Research Laboratory, Electrochemistry Branch, Sensors & Electron Devices Directorate

Ionic liquids are design materials and therefore, they can be adjusted to specific requirements. Due to this fact an understanding on the atomistic scale is helpful to improve ionic liquids with respect to certain properties. To elucidate microscopic processes molecular dynamics (MD) simulations are a powerful tool.

Polarizable force fields for MD simulations are necessary to mimic the electron cloud. Furthermore, they are necessary to produce results which are close to the experiment. In this study, we used an improved version of the APPLE&P force field. The main focus was to investigate different lithium bis(trifluoromethanesulfonyl)imide (TFSI) concentrations in 1-Ethyl-3-Methylimidazolium bis(fluorosulfonyl)imide. The results strongly depend on the lithium salt concentration due to a favored coordination of lithium ions by TFSI.

CPP 22.5 Tue 10:30 PC 203

**Hydrogen Bond Networks in Protic Ionic Liquids** — •Tobias Zentel and Oliver Kühn — Institut für Physik, Universität Rostock

To understand the physico-chemical properties of ionic liquids (ILs), the knowledge of their intermolecular interactions, which is governed by Coulomb and hydrogen bond (HB) interactions, is of utmost importance. The subclass of protic ILs has strong HBs that allow the proton to move from the cation to the anion after an exitation, thus changing the coulombic interactions decisively.

In this contribution we focus on the understanding of the correlations in the HB network dynamics in equilibrium and after excitation of an ion pair. The IL triethylammonium nitrate (tEAN) serves as a convenient example for the investigations, because it features a 'simple' one-dimensional HB network.

The performance, w.r.t describing the HBs in ILs, of density functional based tight binding method (DFTB) is tested by comparing to ab initio simulations. The DFTB method is numerically efficient enough to perform simulations for a box consisting of 24 ion pairs with periodic boundary conditions using equilibrium and non-equilibrium starting structures. The correlated dynamics of the HB and the effect of proton transfers using molecular dynamics is investigated.

CPP 22.6 Tue 10:45 PC 203

**Lattice-Boltzmann simulations of the electrophoretic stretching of polyelectrolytes: The importance of hydrodynamic interactions** — Owen Hickey, Christian Holm, and •Jens Smiatek — Institut für Computerphysik, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

In this talk we examine the electrophoretic stretching of polyelectrolytes between parallel uncharged plates using molecular dynamics simulations. We compare simulations where the fluid is modeled implicitly using a Langevin thermostat, which ignore hydrodynamic interactions, to simulations with an explicit lattice-Boltzmann fluid that take hydrodynamic interactions into account. The difference between simulations with and without hydrodynamic interactions is larger for longer polyelectrolytes, as one would expect. Furthermore, we present simulation results which show that the effects of hydrodynamic interactions are reduced as the distance between the confining plates is diminished. The main result of our study is that hydrodynamic interactions play a larger role in systems with a shorter Debye length, in contrast to conventional wisdom.

CPP 22.7 Tue 11:00 PC 203

**Scaling theory of the counterion-exchange slow mode in salt-free polyelectrolyte solutions** — •Won Kyu Kim and Roland R. Netz — Institut für Theoretische Physik, Freie Universität Berlin, Berlin, Germany

We present a scaling theory for the dielectric response due to the counterion-exchange mode in dilute and semi-dilute polyelectrolyte solutions. The mean escape time for the counterion to cross over the energy barrier between two polyelectrolytes is shown to yield a distinct scaling behaviour, depending on the polyelectrolyte length and the polyelectrolyte monomer concentration, and we discuss the result in connection with the slowest dielectric response in the super-low-frequency mode which was recently found. Including the super-low-frequency mode, we present overall scaling relations of relaxation times in various modes induced by the counterions in the solution, which are in agreement with the experimental results, throughout dilute and semi-dilute regimes. Our results suggest that the counterion-exchange mode may resolve the conflicting theoretical interpretations in the polyelectrolyte dielectric spectroscopy particularly in the low-frequency mode.

CPP 22.8 Tue 11:15 PC 203

**New fitting model for refractive index of PSS/PDADMAC polyelectrolyte multilayers swelling in humid conditions** — •Oliver Löhmann and Regine von Klitzing — Technische Universität Berlin

Polyelectrolyte multilayers (PEMs) are a versatile approach to functionalize charged surfaces. PEMs can be built up by the Layer-by-layer technique which is an easy and well controllable technique to achieve polymer coatings in nanometer range. Polymer coatings are able to respond to external stimuli, e.g. relative humidity (r.h.), depending on their chemical nature. By increasing the r.h., the water uptake can be split into two types of water: the void water which contributes only to changes in the refractive index and the swelling water which changes both, thickness and refractive index. It is still unclear how the voids are filled with water and so far no model for the water adsorption for PEMs exists.

Here, we will present two different fitting models for the refractive index of PEMs in different humidity: The Garnett model and an extended version of the void model. The swelling behavior of PEMs depending on r.h. was measured by Ellipsometry. The PEMs swell in a non-linear behavior and the volume fraction of adsorbed water is independent of the layer number. We will show that the Garnett model only partly describes the refractive index. Taking the filling of voids at low r.h. into account the refractive index in dependence on the r.h. is fully described. Now, it is possible to calculate the volume fraction of air inside the dry PEMs (voids) and the ability of water uptake.

## CPP 23: Interfaces and Thin Films I (joint session CPP, DS)

Time: Tuesday 10:00–12:30 Location: C 243

CPP 23.1 Tue 10:00 C 243

**What is the result of a tensiometer measurement to do with the surface tension?** — •Markus Bier — Max Planck Institute IS and University of Stuttgart, Germany

The surface tension of liquids is routinely measured with various types of tensiometers under ambient pressure conditions [1]. For, e.g., water at room temperture this leads to the well-known value of 0.07 N/m [1]. However, the surface tension is strictly defined only under conditions of liquid-vapour bulk coexistence, whereas, e.g., water at room temperature and ambient pressure is deep in the one-phase region of the phase diagram, far away from phase coexistence. Hence the above-mentioned tensiometer measurements are actually performed at interfaces under non-equilibrium conditions. This leads to the question whether it is legitimate at all to identify the result of a tensiometer measurement of a non-equilibrium interface with the surface tension. This contribution gives an answer to that question [2].

References:
[1] D.R. Lide (ed.), *CRC Handbook of Chemistry and Physics, 82nd edition* (CRC Press, Boca Raton, 2001).
[2] M. Bier and D. Arnold, Phys. Rev. E **88**, 062307 (2013).

CPP 23.2 Tue 10:15 C 243

**Morphometric thermodynamics and interface conventions** — •Andreas Reindl, Markus Bier, and S. Dietrich — Max Planck Institute IS, University of Stuttgart, Germany

Several model fluids with small number densities in contact with planar, spherical and cylindrical walls are investigated within density functional theory. The dependence of the interfacial tension on the curvature of spherical and cylindrical walls is examined and compared to the expression derived within the framework of morphometric thermodynamics. Particular attention is paid to the influence of the choice of the interface location, which underlies the definition of the interfacial tension. We found that morphometric thermodynamics is never exact for the considered systems and that its quality as an approximation depends on the choice of the interface.

CPP 23.3 Tue 10:30 C 243

**The surface tension anomaly of water** — •Marcello Sega[1], George Horvai[2], and Pal Jedlovszky[3] — [1]University of Vienna, Institut für Computergestützte Biologische Chemie, Vienna, Austria — [2]MTA-BME Research Group of Technical Analytical Chemistry, Budapest, Hungary — [3]Department of Chemistry, EKF Training School, Eger, Hungary

The surface tension of water is characterised by an anomalous dependence on the temperature that manifests itself in the form of an inflection point [1]. So far, a microscopic explanation of this phenomenon was missing. By using intrinsic surface analysis on the liquid/vapour interface, simulated using six different water models, we managed to establish a link between the surface tension inflection and the topological properties of the hydrogen-bond network of the surface layer. We discovered that the inflection temperature coincides with the percolation threshold of the hydrogen bond network in the first molecular layer at the liquid/vapour interface. This provides strong evidence that the sudden breakup of the network, which takes place at the percolation threshold, is the underlying microscopic mechanism at the origin of this surface tension anomaly of water [2,3].

[1] J. S. Rowlinson and B. Widom. Molecular Theory of Capillarity; Dover Publications: Mineola, NY, 2002; p 11.

[2] M. Sega, G. Horvai and P. Jedlovszky, Langmuir 30, 2969 (2014)

[3] M. Sega, G. Horvai and P. Jedlovszky, J. Chem. Phys. 141, 054707 (2014)

CPP 23.4 Tue 10:45 C 243

**Liquid drops on a surface: comparing results from microscopic density functional theory (DFT) with mesoscopic modelling and a method for calculating the binding potential** — Adam Hughes[1], Uwe Thiele[2], and •Andrew Archer[1] — [1]Department of Mathematical Sciences, Loughborough University, Loughborough, LE11 3TU, UK — [2]Westfälische Wilhelms-Universität Münster, Institut für Theorestische Physik, Wilhelm-Klemm-Str. 9, 48149 Münster, Deutschland

We present a microscopic DFT based method for calculating the binding potential $g(h)$ for a film of liquid on a solid surface, where $h$ is the thickness of the liquid film. The form of $g(h)$ determines whether or not the liquid wets the surface. We study in detail the effect on $g(h)$ of truncating the range of the dispersion forces, both those between the fluid molecules and those between the fluid and wall. We find this can have a significant effect on the form of $g(h)$ and therefore also on whether the liquid is predicted to wet the surface or not. We also calculate density profiles for liquid drops on a surface, using both DFT and also from inputing $g(h)$ into a mesoscopic free energy. Comparing quantities such as the contact angle and the shape of the drops, we find good agreement between the two methods.

**15 min. break**

CPP 23.5 Tue 11:15 C 243

**Crack-Free Hierarchical Wrinkle Patterns** — •Bernhard Glatz and Andreas Fery — Physical Chemistry II, University of Bayreuth, Universitätsstraße 30, 95447 Bayreuth, Germany

Wrinkling is a mechanical instability phenomenon of thin films: Wrinkles form, if a system consisting of a hard, thin layer in strong adhesive contact with a soft, thick elastomer is subject to in plane compression. Under these conditions, a buckling instability results in a periodic surface corrugation with well-defined wavelength. In that regard PDMS is a well-established elastomer since it allows the in-situ generation of a glassy layer by oxidization processes as plasma or UVO. It comprises however side features as cracks and line defects, which form in most wrinkling process and are not predictable yet. We demonstrate a crack-free method where line defects are arranged by modifying the substrate: A stiffness gradient between two covalently linked PDMS phases induces a change in the wrinkle periodicity along the border of both. We tuned the ratio of the phases and so received several hierarchical line defect patterns. Furthermore computer simulations helped us to understand the observed structures. Such crack-free wrinkles with predictable defect positions allow applications as channel junctions in microfluidics or templates for particle alignment.

[1] B. A. Glatz and co-workers (in preparation)

CPP 23.6 Tue 11:30 C 243

**Condensation of methane in metal organic frameworks (MOFs): Novel phase transitions** — •Nicolas Höft and Jürgen Horbach — Institut für Theoretische Physik II: Soft Matter, Heinrich-Heine-Universität Düsseldorf, Germany

Metal-Organic frameworks (MOFs) are nanoporous crystalline materials where where metal oxide complexes are to connected to each other by organic linkers. Due to the large inner surface, MOFs are well-suited for applications associated with gas adsorption. Experimentally, adsorption isotherms have been studied for molecules such as $CH_4$, $CO_2$, $H_2O$, etc., indicating the possibility of a phase-transition in various MOF structures. However, the nature of these transitions is not well understood, in particular with respect to the interplay between layering on the inner surface and gas-liquid coexistence in the porous structure.

We use grand canonical Monte Carlo simulations in conjunction with successive umbrella sampling to study the condensation of $CH_4$ in the MOF systems IRMOF-1, IRMOF-8, and IRMOF-16. We find a very rich phase behaviour in these systems and analyse in detail the occurring coexisting phases as well as the critical behaviour.

CPP 23.7 Tue 11:45 C 243

**Extreme Surface Propensity of Halide Ions in Water** — •Ellen H.G. Backus[1], Lukasz Piatkowski[2], Zhen Zhang[1], Huib J. Bakker[2], and Mischa Bonn[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]FOM Institute AMOLF, Amsterdam, the Netherlands

The dominant part of water on earth is not pure water; it contains salts. Moreover, especially in atmospheric chemistry the ions present at the interface are important for various reactions occurring at these interfaces. These ions are potentially reactive and/or determine the water structure, thereby influencing the surface reactivity. Experimentally, it is very challenging to determine the local concentration of ions in the outermost molecular monolayer region of aqueous solutions. Here, we show how two-dimensional sum frequency generation spectroscopy can be used to determine this concentration by measuring the energy transfer rate between water molecules. The presence of ions leads to a reduction of this transfer rate. The data reveal a high surface propensity for iodide anions corresponding to a surface concentration three times higher than the bulk concentration.

CPP 23.8 Tue 12:00 C 243

**Pressure induced adsorption of lysozyme at the solid-liquid interface** — •Paul Salmen[1], Julia Nase[1], Susanne Dogan[1], Holger Göhring[1], Irena Kiesel[1,3], Johannes Möller[1,2], Christopher Weis[1], Florian Wirkert[1], Michael Paulus[1], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund, Germany — [2]ESRF - The European Synchrotron, 71 Avenue des Martyrs, F-38043 Grenoble, France — [3]Institut Laue-Langevin, 71 Avenue des Martyrs, 38000 Grenoble, France

The pressure-induced adsorption of proteins at hydrophilic and hydrophobic interfaces was studied by x-ray reflectivity measurements. In our custom-built cell for x-ray reflectivity (XRR) measurements [1], we are able to apply pressures up to 5 kbar and study the solid/liquid interface in-situ with Angstrom resolution. As hydrophobic surfaces, silicon wafers covered with octadecyltrichlorosilane (OTS) were used, while bare silicon wafers with a native silicon dioxide layer provide charged, hydrophilic interfaces. Lysozyme was used in 20 mM BisTris buffer (pH 7.1) at a concentration of 0.1 mg/ml. The measurements were performed at the synchrotron light sources DELTA (Dortmund, Germany), ESRF (Grenoble, France) and SLS (Villigen, Switzerland) using high energy x-ray radiation. At low pressures, only a monolayer of lysozyme adsorbs at both interfaces. When pressure is increased, a second layer of lysozyme adsorbs. Because the thickness of the first layer decreases in this process, we suppose a partial collapse of the first lysozyme layer. [1] F. J. Wirkert et al., Journal of Synchrotron Radiation 2014 (21) doi:10.1107/S1600577513021516

CPP 23.9 Tue 12:15 C 243

**A Standing-Wave Approach in Ambient Pressure Photoemission: Chemical State and Depth Resolved Concentration Profiles of Solid/Liquid and Liquid/Gas Interfaces** — •Slavomir Nemsak[1], Hendrik Bluhm[2], Charles Fadley[3], and Claus Schneider[1] — [1]Peter Grünberg Institut 6, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Chemical Sciences Division, Lawrence Berkeley National Laboratory, 94720 Berkeley, CA, USA — [3]Department of Physics, University of California, 95616 Davis, CA, USA

A standing wave approach in the ambient pressure photoelectron spectroscopy is a new and powerful technique to study heterogeneous processes in solid/gas, liquid/gas and solid/liquid interfaces [1]. Advantages of the technique, such as superb depth resolution and chemical sensitivity, are demonstrated on several model systems with relevance to energy research, heterogeneous catalysis, electrochemistry, and atmospheric and environmental science. A strong standing-wave is generated using a multi-layer Si/Mo mirror as a substrate and phase of the standing wave is tailored through the interface of interest by rocking the sample around the Bragg angle. Photoemission signal from different species is then analyzed in order to provide their spatial arrangement, as well as local potential variations, along the direction perpendicular to the interface with sub-nm accuracy. Pros and cons of using harder X-ray excitation are discussed in terms of a photoemission signal strength and a standing wave effects amplitude.

[1] Nemsak et. al, Nature Communications 5, 2014.

# CPP 24: Focus session: Structure, chemistry, and ion solvation at solid-liquid interfaces I (joint session O, CPP)

Time: Tuesday 10:30–12:30 Location: HE 101

**Topical Talk** CPP 24.1 Tue 10:30 HE 101

**Water adsorption on Ru(0001): A molecular perspective** — •Sabine Maier — Department of Physics, FAU Erlangen-Nürnberg, Germany

Water and its dissociation products play an important role in many areas of fundamental science and technological applications. The water molecules at the interface with metal surfaces are arranged differently than those in the bulk liquid or ice due to their strong bonding to the surface. Here, molecular level studies are presented using low temperature scanning tunneling microscopy, that offer new insights into the formation of a wetting layer and the water dissociation process on Ru(0001). We found a bonding motif of the first water layer consisting of rotated hexagonal molecular domains connected by pentagons and heptagons, which deviates significantly from the conventional ice-like water model.[1] Above 150K, we observed the formation of mixed water-hydroxyl structures following partial dissociation. The reaction path for the dissociation process and its energetics will be discussed.[2]

[1] S. Maier et al. Phys. Rev. B 85, 155434 (2012)

[2] S. Maier et al. Phys. Rev. Lett. 112, 126101 (2014)

CPP 24.2 Tue 11:00 HE 101

**Probing Water Structure at the $\alpha$-Al$_2$O$_3$(0001) Surface Using Interface Specific Vibrational Dynamics** — Yujin Tong, Harald Kirsch, Martin Wolf, and •R. Kramer Campen — Fritz-Haber-Institut, Abt. Physikalische Chemie, 14195 Berlin, Germany

$\alpha$-Al$_2$O$_3$(0001) surfaces exposed to water are ubiquitous in engineered applications and a useful model for more complicated alumino-silicate surface/water interaction omnipresent in the environment. Despite this ubiquity, gaining a molecular level understanding of water $\alpha$-Al$_2$O$_3$(0001) interaction has proven challenging. It has recently been proposed, based partly on simulation, that the first layer of water on this surface is essentially hydrophobic: while hydrogen bonding occurs within this first layer, neither surface aluminols nor the first layer of molecular water donate a hydrogen bond to overlying bulk liquid. Direct experimental evidence for such a non-wetted water layer has thus far proven elusive. Here we probe the existence of this layer using interface specific vibrational relaxation as a probe of surface water structure. We find, using an ultrafast time resolved infrared pump - vibrational sum frequency probe scheme, that the T$_1$ of OH groups at the $\alpha$-Al$_2$O$_3$(0001) surface is $\approx$ 8 ps: intermediate between that of surface aluminols in contact with excess water ($<$ 1 ps) and that of isolated surface OH groups on oxide surfaces ($>$ 100 ps). This intermediate T$_1$ is the first direct experimental insight consistent with a non-wetted interfacial water layer on the $\alpha$-Al$_2$O$_3$(0001) surface.

CPP 24.3 Tue 11:15 HE 101

**A joint *first principles* and ATR-FTIR study of the vibrational properties of interfacial water at Si(100):H-H$_2$O solid-liquid interfaces** — •lei yang[1], stefanie tecklenburg[1], andreas erbe[1], stefan wippermann[1], francois gygi[2], and giulia galli[3] — [1]Max-Planck-Institute for Iron Research, Duesseldorf, Germany — [2]University of California, Davis, Davis, United States — [3]University of Chicago, Chicago, United States

Understanding the structural and bonding properties of solid-liquid interfaces is crucial for a wide range of (photo-)electrochemical applications, such as e. g. solar water splitting and electrolysis. However, there are no experimental techniques presently available allowing one to directly probe the microscopic structure of solid-liquid interfaces. We present a joint investigation of the vibrational properties of interfaces between liquid water and prototypical semiconductor substrates, i.e. hydrogenated silicon surfaces. We carried out (ATR-FTIR) spectroscopy measurements and *ab initio* molecular dynamics simulations. The latter allowed us to interpret the experiments and to unravel specific bonding configurations and interactions of water molecules with the solid surfaces. Our study highlights the key role of coupled theory-experimental investigations on well controlled and characterized interfaces, in order to develop robust strategies to interpret experiments and validate theory. This work provides a solid basis for investigating ion solvation and chemical processes at the interface. G. G. and F. G. acknowledge DOE-BES Grant No. DE-SS0008939.

**Topical Talk** CPP 24.4 Tue 11:30 HE 101

**Using resonant inelastic soft x-ray scattering maps to study liquids, gases, and their interfaces** — •Lothar Weinhardt — IPS, Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany — ANKA Synchr. Radiation Facility, KIT, Eggenstein-Leopoldshafen, Germany — Dep. of Chem., University of Nevada, Las Vegas, U.S.A. — ITCP, KIT, Karlsruhe, Germany

X-ray emission spectroscopy (XES) and Resonant Inelastic X-ray Scattering (RIXS) have recently been applied to study liquid and gaseous systems. Such experiments became possible with new specialized experimental setups and given a unique insight into the electronic and vibrational structure of these systems. In this way, information on solvent/solute interactions, hydrogen bonding, molecular symmetries, excited-state dynamics, and many other aspects could be gathered. Finally, interfaces between solids and a gas/liquid can be studied in an in-situ fashion, which is of particular relevance for a wide range of applied systems including catalysis, electrochemistry, or the influence of environmental conditions on surfaces. In this presentation, we will report on our recent progress on studying such systems using XES and RIXS. By the development of a high-transmission soft x-ray spectroscopy setup we are able to measure complete Resonant Inelastic soft X-ray Scattering (RIXS) maps. These maps give a comprehensive picture of the electronic structure of occupied as well as unoccupied electronic states of the studied system. We will demonstrate the power of this approach by discussing the results obtained on selected liquids, gases, solutions, as well as gas/solid- and liquid/solid interfaces.

**Topical Talk** CPP 24.5 Tue 12:00 HE 101

**Effect of flow on water organization at solid interfaces** — •Mischa Bonn — Max Planck Institute for polymer research, Mainz, Germany

At the surface or interface of water, the water hydrogen-bonded network is abruptly interrupted, conferring properties on interfacial water different from bulk water. Owing to its importance for disciplines such as electrochemistry, atmospheric chemistry and membrane biophysics, the structure of interfacial water has received much attention.

We elucidate the structure and structural dynamics of interfacial water using ultrafast surface-specific sum-frequency generation (SFG) vibrational spectroscopy. We make use of the fact that the SFG signal depends critically on the interfacial organization of water molecules. We attempt to bridge continuum models of laminar flow along interfaces, with molecular-level descriptions of the Stern and diffuse layer, which describe the near-surface distribution of ions.

For water at two different mineral interfaces, we report a dramatic effect of water flow water along the mineral surface on the organization of water at the interface. Our observations can be explained by considering the coupling between the flow and the dissolution chemistry at the interface. Even for low-soluble quartz at neutral pH, dissolution plays a key role in determining the interfacial water organization.

# CPP 25: Focus session: Structure, chemistry, and ion solvation at solid-liquid interfaces II (joint session O, CPP)

Time: Tuesday 14:00–16:00 Location: HE 101

**Topical Talk** CPP 25.1 Tue 14:00 HE 101

**First-Principles Microkinetic Modeling at Solid-Liquid Interfaces: First Steps** — •Karsten Reuter — Technische Universität München, Germany

Over the last decade first-principles based microkinetic models have become a common tool to describe solid-gas processes like heterogeneous catalysis or crystal growth. For processes at solid-liquid interfaces such modeling is in its infancy. Challenges arise already in the efficient treatment of solvation effects or in the determination of individual rate constants, where extended time-scale simulations are required to capture the often complex and rough free energy barriers.

In this talk I will review our first steps to address corresponding challenges, focusing on water/aspirin as a showcase application. For corresponding active pharmaceutical ingredients knowledge of their intrinsic dissolution rates is a cornerstone to optimize the pharmacokinetics. We achieve this goal within a spiral-growth microkinetic model that draws on dissolution rate constants obtained within a novel hyperdynamics-metadynamics molecular simulation approach.

**Topical Talk** CPP 25.2 Tue 14:30 HE 101

**Structure of metal electrode-electrolyte interfaces determined from first principles** — •Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany — Helmholtz Institut Ulm - Elektrochemische Energiespeicherung, 89069 Ulm, Germany

The theoretical description of electrode-electrolyte interfaces from first principles is hampered by the complexity of the interface structures and the liquid nature of the electrolyte requiring computationally expensive statistical averaging. Despite these obstacles, significant progress has been made in the modeling in recent years. In this contribution, I will present our attempts to contribute to this progress by systematically increasing the complexity of the considered systems [1, 2]. The electrolyte can be described either as a thermodynamic reservoir or using implicit of explicit solvent models. Using these approaches, the equilibrium coverage of specifically adsorbed anions such as halides as a function of the electrode potential will be addressed. This represents an integral part of the realistic modeling of electrochemical double layers. Additionally, on metal electrodes such as platinum the adsorption of H or OH - depending on the electrode potential - has to be considered in the presence of an aqueous electrolyte. Finally, the structure of organic electrolytes on metal electrodes that is governed by weak dispersion forces will be discussed [2, 3].

[1] Axel Groß *et al.*, J. Electrochem. Soc. **161**, E3015 (2014).
[2] Nicolas Hörmann *et al.*, J. Power Sources **275**, 531 (2015).
[3] F. Buchner *et al.*, ACS Nano **7**, 7773 (2013).

**Topical Talk** CPP 25.3 Tue 15:00 HE 101

**Synchrotron x-ray determination of ion distributions at liquid interfaces** — •Jean Daillant — Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, BP48, F-91192 Gif sur Yvette Cedex, France

The interfacial behavior of ions is of key importance in a number of phenomena ranging from microfluidics to chemistry in the atmosphere and from protein stability to the transport of pollutants in water.

Beyond Coulombic interaction, the polarisability and hydration of the ions as well as water interfacial structure are important, leading to ion specificity, i.e. possibly dramatically different behavior for ions like $Cl^-$ and $I^-$. Understanding these effects requires measurements to access the surface composition at the relevant nanometric length-scale.

Investigating the surface composition of alkali-halide aqueous solutions using grazing incidence x-ray fluorescence, differences in concentration over a few angstrom could be resolved, with, for example $I^-$ or $Br^- > Cl^-$. These results could be explained by including a short-range potential accounting for short-range solvent mediated couplings.

Polarization of the liquid-Hg aqueous electrolyte induces extremely large decrease in surface energy with strong ion specificity. Using x-ray reflectivity, we could determine the interfacial structure, demonstrating an accumulation of ions at the Hg surface. Our results challenge the long-standing approximation that assimilates the Hg surface to a smooth, chemically inert surface with a uniform surface charge density.

Finally, using the standing wave technique which allows both high spatial and element sensitivity, we have investigated ion distributions in nano-channels, and I will discuss the first results we have obtained.

**Topical Talk** CPP 25.4 Tue 15:30 HE 101

**Modelling of electrical double layers at metal oxide electrodes** — •Michiel Sprik[1] and Jun Cheng[2] — [1]Department of Chemistry, University of Cambridge, Cambridge UK — [2]Department of Chemistry, University of Aberdeen, Aberdeen, UK

Oxide surfaces exchange protons with an aqueous electrolyte and can therefore carry a net proton charge. The adsorbed protons at low pH can be partially or fully discharged by conduction electrons or the deprotonated anionic groups at high pH by holes. The "intrinsic" equilibrium constants for this process (acidities, ionization and dehydrogenation free energies) can be computed for charge neutral surfaces. We have developed such a method using Density Functional Theory based Molecular Dynamics (DFTMD, for an application to rutile titania see Angew Chem Int Ed Engl (2014) 53, 12046). An electrode with net excess or deficit proton charge can be described in first approximation by a triple layer model consisting of the charged electrode surface, ionic counter charge on the electrolyte side (a Helmholtz layer at high ionic strength) and a space charge layer on the electrode side. After a summary of our DFTMD method, we will outline in this talk how the equilibrium constants computed by the DFTMD simulation can be used in an analytic model for an "electron coupled proton adsorption isotherm". The additional parameter in this model is the capacitance of the Helmholtz layer. Such a parametrized isotherm should enable us to analyse the effect of double layers on the (photo) electrocatalytic properties of metal oxides as will be shown for the example of the oxidation of adsorbed water molecules.

# CPP 26: Organic Electronics and Photovoltaics: OPV I (joint session CPP, HL, TT)

Time: Tuesday 14:00–16:00 Location: C 130

**Invited Talk** CPP 26.1 Tue 14:00 C 130

**Ultrafast Coherent Charge Transfer in Solar Cells and Artificial Light Harvesting Systems** — •Christoph Lienau[1], Ephraim Sommer[1], Antonietta de Sio[1], Ralf Vogelgesang[1], Margherita Maiuri[2], Giulio Cerullo[2], Angel Rubio[3], Carlo A. Rozzi[4], and Elisa Molinari[4] — [1]Carl von Ossietzky University, Oldenburg, Germany — [2]Politecnico di Milano, Milano, Italy — [3]Universidad del País Vasco, San Sebastian, Spain — [4]Dipartimento di Scienze Fisiche, Modena, Italy

To elucidate the fundamental microscopic processes in solar energy conversion, we have recently combined coherent femtosecond spectroscopy and first-principles quantum dynamics simulations [1,2] and have used this approach to explore the primary photoinduced electronic charge transfer in two prototypical structures: (i) a carotene-porphyrin-fullerene triad, an elementary component for an artificial light harvesting system [2] and (ii) a polymer:fullerene blend as a model for an organic solar cell [1].

Our results provide strong evidence that in both systems, at room temperature, the driving mechanism of the primary step within the current generation cycle is a quantum-correlated wavelike motion of electrons and nuclei on a timescale of few tens of femtoseconds. They suggest that the strong coupling between electronic and vibrational degrees of freedom is of key importance for the dynamics and yield of the charge separation process. Here, I will discuss our most recent experimental and theoretical findings. [1] S. M. Falke et al., Science 344, 6187 (2014). [2] C. A. Rozzi et al., Nature Comm. 4, 1602 (2013)

CPP 26.2 Tue 14:30 C 130

**Calculation of exciton dissociation rates in ordered and disordered 2D model organic photovoltaic interfaces** — •Hector Vazquez[1] and Alessandro Troisi[2] — [1]Inst. of Physics, Academy of Sciences of the Czech Rep., CZ — [2]Dept. of Chemistry and Centre of Scientific Computing, University of Warwick, UK

The efficient generation of free charges from incident light in organic photovoltaic cells has been studied extensively but is not yet well understood. In order to separate, electron and hole have to overcome the Coulomb attraction and several mechanisms have been proposed. In particular, 'hot' excitons having excess energy have received a lot of attention but no consensus yet exists [1].

In this talk, I will introduce a method to calculate exciton dissociation rates [2] and will describe its application to 2-Dimensional model organic photovoltaic interfaces. The method uses Green's functions within a widely applicable model Hamiltonian of donor/acceptor interfaces with and without disorder. Initial states are Frenkel excitons while final states are Charge-Transfer (CT) states. I will present results for the generation rates of CT states where I will highlight the importance of disorder and the delocalization of the excitonic wavefunctions. Excitons dissociate into 'hot' CT states with partially separated charges, where electron and hole are located far from the interface.

1) A. A. Bakulin et al., Science 335, 1340 (2012), A. E. Jailaubekov et al., Nat. Mater. 12 66 (2013), G. Grancini et al., Nat. Mater. 12 29 (2013), K. Vandewal et al., Nat. Mater. 13 63 (2013).

2) H. Vazquez, A. Troisi, Phys. Rev. B 88, 205304 (2013).

CPP 26.3 Tue 14:45 C 130

**Charge separation at $C_{60}$/P3HT and P3HT/ZnO interfaces probed by femtosecond time-resolved second harmonic generation measurements** — •Marc Hänsel[1], Michael Schulze[1], Yunus Sevinchan[2], Yana Vaynzof[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, Heidelberg, Germany — [2]Centre of Advanced Materials, Heidelberg, Germany

A deeper understanding of the process of ultrafast charge transfer and separation at donor/acceptor interfaces is a prerequisite for improvement of organic and hybrid solar cells. Time-resolved second harmonic generation (TR-SHG) with femtosecond temporal resolution was used to investigate different donor/acceptor interfaces. With this intrinsically interface sensitive technique we were able to monitor the charge transfer dynamics of the well-defined single heterojunctions $C_{60}$/P3HT and P3HT/ZnO. In addition some modifications via cesium doping were made to the ZnO/P3HT interface. At the $C_{60}$/P3HT interface a pump energy dependent ultrafast charge transfer state with a population time of 320fs has been observed.

CPP 26.4 Tue 15:00 C 130

**Modelling charge transfer in Polymer/SWNT/PCMB hybrid systems** — •Livia Glanzmann, Duncan Mowbray, and Angel Rubio — Nano-bio Spectroscopy Group and ETSF Scientific Development Centre, Universidad del Pais Vasco UPV/EHU, Av. Tolosa 72, E-20018 San Sebastian, Spain

One way to increase power conversion efficiencies of organic photovoltaic devices (OPVs) is to optimize the electron donor (D) acceptor (A) materials. The level alignment of the frontier orbitals at the D-A heterojunction interface is important for an efficient charge transfer. Since the first heterojunction OPV, consisting of 3-alkylpolythiophene (P3HT) and Fullerene, several combinations of D-A materials were tested. As well, carbon nanotubes were introduced, which increased the efficiency of such multi-component systems. Still, the electronic processes within such systems are not well understood. To shed light on this subject, we simulate photovoltaic processes occuring in selected sets of P3HT-based-Polymer/SWNT or PCBM heterojunctions. As a first step, we create the excited states within the donor materials by performing TDDFT calculations and extract the electron density of the exciton. Then, we use the delta SCF approach to study the D-A electron transfer. On top, we calculate the probability of an electron passing the D-A interface and being transported through a nanotube by performing G0W0 calculations. All these results show the effect of certain types of D-A material, as well of their level alignment, on the efficiency of OPVs.

CPP 26.5 Tue 15:15 C 130

**Photoinduced Dynamics of Charge Separation: from Photosynthesis to Polymer-Fullerene Bulk-Heterojunctions** — •Andreas Sperlich[1], Oleg G. Poluektov[2], Jens Niklas[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Chemical Sciences and Engineering Division, ANL, Argonne, Illinois 60439, USA — [3]ZAE Bayern, 97074 Würzburg

Understanding charge separation and charge transport is crucial for improving the efficiency of organic solar cells. This is due to the excitonic nature of their active media, based on organic molecules, serving as both a light absorbing and transport layer. Charge transfer (CT) states play an important role, being intermediate for free carrier generation and charge recombination. Here, we use light-induced electron paramagnetic resonance (EPR) spectroscopy to study the charge transfer dynamics in composites of the polymers P3HT, PCDTBT, and PTB7 with the fullerene derivative $PC_{60}$BM. Transient EPR measurements show strong spin-polarization patterns for all polymer-fullerene blends, confirming predominant generation of singlet CT states. These observations allow a comparison with charge separation processes in molecular donor-acceptor systems, as found in natural and artificial molecular photosynthetic systems and clarification of the initial steps of sequential charge transfer in organic photovoltaic (OPV) materials. The detection of strong electron spin-polarization in OPV materials points out to the significance of spin dynamics for the efficient functioning of solar cell devices.

CPP 26.6 Tue 15:30 C 130

**Sub-ns Triplet State Formation in PSBTBT:PC70BM and PCPDTBT:PC60BM Photovoltaic Blends** — Fabian Etzold[1], Ian Howard[1,2], and •Frédéric Laquai[1] — [1]Max Planck Research Group for Organic Optoelectronics, Max Planck Institute for Polymer Research, D-55128 Mainz, Germany — [2]Institute of Microstructure Technology (IMT), Karlsruhe Institute of Technology (KIT), D-76344 Eggenstein-Leopoldshafen, Germany

The excited state dynamics in low-bandgap polymer:fullerene blends using the donor-acceptor copolymers PCPDTBT and its silicon-substituted analogue PSBTBT are investigated by femto- to microsecond broadband Vis-NIR transient absorption (TA) pump-probe spectroscopy. The TA experiments and analysis of the TA data by multivariate curve resolution (MCR-ALS) reveal that after exciton dissociation and free charge formation is completed, fast sub-nanosecond non-geminate recombination occurs and leads to a substantial population of the polymer's triplet state. The extent to which triplet states are formed depends on the initial concentration of free charges, which itself is controlled by the microstructure of the blend, especially in case of PCPDTBT:PC60BM. Interestingly, PSBTBT:PC70BM blends show a higher charge generation efficiency, but less triplet state formation at similar free charge carrier concentrations. This indicates that the solid-state morphology and interfacial structure of PSBTBT:PC70BM blends reduce non-geminate recombination and thus triplet state formation, leading to increased device performance compared to optimized PCPDTBT:PC60BM blends.

CPP 26.7 Tue 15:45 C 130

**Triplet Exciton Formation in High-Efficiency Donor-Acceptor Photovoltaic Blends** — •Stefan Väth[1], Hannes Kraus[1], Andreas Baumann[2], Kristofer Tvingstedt[1], Andreas Sperlich[1], Vladimir Dyakonov[1,2], John Love[3], and Thuc-Quyen Nguyen[3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg — [3]University of Santa Barbara, Santa Barbara, CA 93106, USA

In donor-acceptor based bulk-heterojunction solar cells, the splitting of singlet excitons at the donor and acceptor interface is of crucial importance for charge generation. The reversed process, in which two initially free charge carriers meet at the interface to form an exciton with singlet or triplet multiplicity is rather beneficial for light emission in OLEDs but considered as one of the loss factors in OPV.

In our experiments, the occurrence of triplet excitons and CT states was probed by using spin sensitive detection of the photo- and electroluminescence. A substantial generation of molecular triplet excitons was found in high efficiency donor-acceptor OPV systems based on the low bandgap copolymer PTB7 and in the soluble small molecule p-DTS(FBTTh2)2, both blended with PC70BM as acceptor. We ascribe these findings to an electron back transfer from the CT state to the triplet state on the donor material. In summary, the fundamental understanding of the transformation processes involving the CT states, triplet excitons, as well as free electrons and holes and their dependence on nanoscale morphology and energetics of blends is essential for the optimization of OPV devices.

# CPP 27: Interfaces and Thin Films II (joint session CPP, DS)

Time: Tuesday 14:00–16:00 Location: C 243

**Invited Talk** CPP 27.1 Tue 14:00 C 243

**Structure formation at interfaces: breath figures and beyond** — •Masoud Amirkhani — Institut für Experimentelle Physik Universität Ulm Albert-Einstein-Allee 11 89081 Ulm, Germany

The interaction of two (or more) different materials in contact is crucial for basic science as well as for practical purposes. At the micro and nano regime, the number of molecules at the interface is comparable to that of bulk molecules so the interaction at the interface governs the overall structure and functionality of the system. The interface interaction is particularly crucial for the formation of emulsions, microemulsions and surface micelles. Additionally, the existence of a large interface does directly affect the adsorption of polymer on the surface and the performance of many systems such as ionic polymer metal composites (IPMC). One should note that the interface interaction can be altered using various physical and chemical stimuli. For example amphiphilic and amphiphilic-like molecules are able to modify surfaces and interface properties and also form self-assembled structures. In this talk, we present the investigation of the size and structure of surface emulsion and microemulsions under the influence of different additives. Additionally, the conformation and configuration of diblock copolymer on the substrate under the influence of solvent vapor annealing and electric field will be discussed.

CPP 27.2 Tue 14:30 C 243

**Simulations of solvent vapor annealing of cylinder-forming blockcopolymer thin films** — •Anatoly V. Berezkin[1], Igor I. Potemkin[2], and Christine M. Papadakis[1] — [1]Technische Universität München, Physik Department, München, Germany — [2]Lomonosov Moscow State University, Physics Department, Moscow, Russian Federation

Ordered block copolymer films are promising as functional templates for lithography, molecular biology, colloid science etc. Using dissipative particle dynamics, we simulated the solvent vapor annealing (SVA) that is used to relax morphological defects, and control domain orientation in these films. The drying of films was considered in case of intermediate A/B block segregation and fast solvent evaporation. Under these conditions, the SVA transforms equilibrium morphology of lying cylinders to hexagonally ordered perpendicular cylinders in the wide parameter range. The best conditions for this were a moderate initial solvent concentration in the film, and a selectivity of the solvent to the major block. This is probably necessary to compensate entropy-driven adsorption of the short blocks at the film surfaces, revealed in other works. Too weak or too strong block segregation, or solvent selectivity result in disordered morphologies. First disordered microdomains are formed, and than after evaporation of the half of the solvent, the domains reorient along the gradient of solvent concentration. This may be explained by the Gibbs-Marangoni effect. Such mechanism of microdomain ordering notably distinguishes from those observed in other recent simulations.

CPP 27.3 Tue 14:45 C 243

**Instabilities in PS-PVP polymer blends thin films driven by surface tension and temperature effects** — •Marlena Filimon[1], Jean-Nicolas Audinot[2], Patrick Grysan[2], Jörg Baller[1], and Roland Sanctuary[1] — [1]Laboratory for the Physics of Advanced Materials, University of Luxembourg, Luxembourg — [2]Department of Science and Analysis of Materials , Centre de Recherche Public-Gabriel Lippmann, Belvaux, Luxembourg

In thin supported films of polymer blends, in addition to composition and molecular weight of components, the structure is dependent on the surface energies of the components and on geometrical constraints induced by confinement in a thin film. Two-dimensional patterns attributed to the Marangoni instability and dependence of the Gibbs free energy of mixing components were observed for a interesting polymer blend ( polystyrene/poly(vinylpyrollidone) (PS-PVP)) thin films. As tools for investigating the nano-size domains structures of thin polymer blends (~150 nm) , we exploited Tapping-Mode Atomic Force Microscopy (TM-AFM) and Nano-dynamic Secondary Ion Mass Spectrometry technique (Nano-SIMS 50. Additionally, wetting properties of the substrate and influences of these instabilities are studied using wetting measurements - contact angle. We propose a possible formation mechanism for presented patterns and show that the mechanism is relevant to the Marangoni instability. The relevant variables which can affect the morphological evolution such as surface enrichment and temperature dependence were also discussed.

CPP 27.4 Tue 15:00 C 243

**Morphological Changes of Surface Immobilized Responsive Micelles** — •Inna Dewald[1], Julia Gensel[1], Johann Erath[1], Eva Betthausen[2], Axel H. E. Müller[2,3], and Andreas Fery[1] — [1]University of Bayreuth, Physical Chemistry II — [2]University of Bayreuth, Macromolecular Chemistry II — [3]Johannes Gutenberg University Mainz, Institute of Organic Chemistry

In recent years, formation of a multitude of smart coatings made from macromolecular building blocks has been demonstrated. Typical examples are brush type architectures or films formed by layer-by-layer self assembly (LbL-SA). In our work, we investigate multicompartment micelles formed from amphiphilic ABC triblock terpolymers as building blocks for responsive coatings. The application of such colloidal units for thin films has several advantages from a material-science perspective, e.g. stimulus-responsivity and multi-functionality on a single particle level and simple preparation of coatings by physisorption. Besides, using LbL-SA allows forming hierarchically structured coatings with novel properties and collective stimulus response of the integrated nanostructures.[1] Here, we investigate the effects of pH and salt on properties of these films [2] and explore the accompanying morphological changes of the surface immobilized micelles as a function of their composition, i.e. properties of each block and the succession they are connected to each other. 1.Gensel J., Dewald I., Erath J., Betthausen E., Müller A. H. E., Fery A., Chem. Sci., 2013, 4, 325. 2.Gensel J., Betthausen E., Hasenöhrl C., Trenkenschuh K., Hund M., Boulmedais F., Schaaf P., Müller A. H. E. and Fery A., Soft Matter, 2011, 7, 11144.

CPP 27.5 Tue 15:15 C 243

**Polymer-solid interphases and glass transition probed by positron annihilation lifetime spectroscopy** — Christian Ohrt, Tönjes Koschine, •Klaus Rätzke, and Franz Faupel — University of Kiel, Chair for Multicomponent Materials, D-24143 Kiel, Germany

The properties of materials involving polymer-solid interfaces are not only determined by the constituents but also by the interfacial region of the polymer near the solid, the so-called interphase. This interphase is particularly important in polymer-based nanocomposites. Here we report on positron annihilation lifetime spectroscopy (PALS) measurements of the free volume near the interface with a moderated positron beam. First investigations from the polymer side indicated a reduced free volume in Teflon AF / Si samples [1] but no quantitative information. Analysis from substrate side with a focused beam through a hole showed a significant average density increase iin an interphase region with a width of about 10 nm. Additionally, the glass transition temperature as a probe for chain dynamics was determined as function of distance to the interface in a Teflon AF / SiN sample with depth resolved PALS. Within error margins, no change in the glass transition temperature could be detected in the interfacial region.

[1] S. Harms, K. Rätzke, V. Zaporojtchenko, F. Faupel W. Egger, L. Ravelli, Polymer, 52 (2011) 505

CPP 27.6 Tue 15:30 C 243

**Conjugated diblock copolymer/fullerene bulk heterojunction system in organic photovoltaic application** — •Rui Wang[1], Zhenyu Di[1], Henrich Frielinghaus[1], Peter Müller-Buschbaum[2], and Dieter Richter[1] — [1]Jülich Center for Neutron Science, outstation at FRM II, Lichtenbergstr. 1, 85747 Garching — [2]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

In order to achieve an optimum energy conversion efficiency for polymer based organic solar cells an interpenetrating bulk heterojunction (BHJ) network is needed, which has a nanoscale morphology on the order of the exciton diffusion length. The interpenetrating network provides larger interface area for exciton dissociation as well. Diblock copolymers are very promising for achieving well controlled nanoscale morphologies. In the present work, we blend the conjugated diblock copolymer P3HT-b-PS with the fullerene derivative PCBM. By applying grazing incidence small angle neutron scattering (GISANS) we investigate the active layer, GISANS had proven to give good contrast conditions for polymer:PCBM films in previous investigations. We present the determined structures in terms of phase information, size of structural length scales and molecular miscibility between the components.

CPP 27.7 Tue 15:45 C 243

**Controlling Nanostructures by Templated Templates: Inheriting Molecular Orientation in Binary Heterostructures** — •Tobias Breuer and Gregor Witte — AG Molekulare Festkörperphysik, Philipps-Universität Marburg, Deutschland

Precise preparation strategies are required to fabricate nanostructures of specific arrangement. In bottom-up approaches, where nanostructures are gradually formed by piecing together individual parts to the final structure, the self-ordering mechanisms of the involved structures are utilized. In order to achieve the desired structures regarding morphology, grain size and orientation of the individual moieties, templates can be applied, which influence the formation process of subsequent structures. However, this strategy is of limited use for complex architectures, as the templates only influence the structure formation at the interface between the template and the first compound. Here, we discuss the implementation of so-called templated templates and analyze, in which extent orientations of initial layers are inherited in top layers of another compound to enable structural control in binary heterostructures. To that purpose we have prepared crystalline templates of the organic semiconductors pentacene and perfluoropentacene in different exclusive orientations. We observe that for templates of both individual materials the molecular orientation is inherited in the top layers of the respective counterpart.

## CPP 28: New Instruments and Methods

Time: Tuesday 14:00–16:00 Location: C 264

CPP 28.1 Tue 14:00 C 264

**New spectroscopic approaches for periodic systems** — •Sandra Luber — Universität Zürich, Institut für Chemie, Winterthurerstr. 190, 8057 Zürich, Schweiz

Knowledge about local properties is extremely helpful for the analysis of structures and interactions. Moreover, it is a valuable source of information for the characterisation of dynamic processes and facilitates the interpretation of experimental data. In case of vibrational spectroscopy, for example, it is desirable to determine the impact of certain atoms/molecules on the bands in the experimental spectra. This may be straight forward for small systems but becomes more and more complex for larger systems.

Calculations provide additional insight allowing the targeted study of specific structures. In this way, it is possible to quantify the contributions of solute and solvent molecules [1] or adsorbates on solids.

We present novel, computationally efficient methods for the calculation of properties for periodic systems such as liquids and solids. These are applied to calculate, among others, vibrational spectra via ab initio molecular dynamics [2,3].

References:

[1] S. Luber, J. Phys. Chem. A 117 (2013) 2760. [2] S. Luber, M. Iannuzzi, J. Hutter, J. Chem. Phys. 141 (2014) 094503. [3] S. Luber, submitted.

CPP 28.2 Tue 14:15 C 264

**Combination of 3D-cross correlated light scattering with small-angle neutron scattering: PNIPAM microgel particles as model system** — •Annegret Günther[1,2], Yvonne Hertle[1], Daniel Clemens[2], Johannes Bookhold[1], Fangfang Chu[2], Matthias Ballauff[2], and Thomas Hellweg[1] — [1]Universität Bielefeld, PCIII, Universitätsstr. 25, 33615 Bielefeld — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, EM-ISFM, Hahn-Meitner-Platz 1, 14109 Berlin

The combination of 3D-cross correlation light scattering (3D-LS) with small-angle neutron scattering (SANS) will enable researchers, particularly in the field of soft condensed matter, to perform simultaneously neutron and light scattering experiments on highly concentrated samples. In order to show the applicability of this new setup PNIPAM microgel particles were used as a model system. For this kind of 'smart material' it was shown [1], that these particles in solution are deformed at higher particle concentrations. Since conventional light scattering experiments have to be performed on diluted samples to assure that only single-scattered light is detected, this concentration effect could only be observed by SANS. 3D-LS suppress the multiple scattering by performing two simultaneously light scattering experiments. By combining the 3D-LS with the SANS instrument V16 at the Helmholtz-Zentrum in Berlin, it will be possible to study samples under exact the same conditions for both scattering experiments.

[1] M. Stieger, J. S. Pedersen, P. Lindner and W. Richtering, Langmuir 20, 7283 (2004).

CPP 28.3 Tue 14:30 C 264

**Non-destructive methods to determine the degree of crosslinking in polymeric materials** — Gabriele Eder and •Volker Uhl — Austrian Research Institute for Chemistry and Technology (OFI), Vienna, Austria

The degree of crosslinking of many polymeric materials has a high impact on some technically important physical properties like hardness, elasticity, ductility or solubility. The main task of the work presented is to show that several quick and non-destructive characterization methods suited to determine the degree of crosslinking of polymeric component parts can be directly used to derive technically relevant physical or mechanical parameters. This can be achieved when a direct correlation between the measured and the physical properties of interest exist. As example, two series of variably cross-linked HDPE components were chosen, a material widely used for tubings and pipes, and investigated with various non-destructive methods. NIR-spectroscopy, confocal Raman spectroscopy and scanning acoustic microscopy proved to yield measured quantities directly correlated to the dose of irradiation used to crosslink the polymer. The results of these methods were validated against crosslinking data determined with conventional chemical analysis based on the solubility of the polymer. Furthermore, the degree of crosslinking was put into relation to characteristic mechanical parameters like Young's modulus and tensile strength, which were determined by mechanical testing.

CPP 28.4 Tue 14:45 C 264

**Fiber enhanced Raman sensing of pharmaceutical drugs** — •Torsten Frosch[1,2], Di Yan[1], and Juergen Popp[1,2] — [1]Leibniz Institute of Photonic Technology — [2]Institute of Physical Chemistry, Friedrich Schiller University Jena

Raman spectroscopy provides excellent molecular sensitivity for the analysis of pharmaceutical drugs and can also be applied in aqueous and biological environments. However the inelastic scattering process lacks high sensitivity. This drawback can be circumvented with help of innovative micro-structured hollow core fibers [1-3]. Such hollow fibers provide a miniaturized sample container for analyte flow and act at the same time as optical waveguide. Thus a very efficient interaction of the analyte molecules and the laser was achieved and the analytical sensitivity was highly improved for tracing molecules at very low concentrations [1]. Fiber enhanced Raman spectroscopy (FERS) was for the first time extended in the important UV spectral range1 and new concepts for optical waveguides in the deep UV were developed [2].

Acknowledgment: Funding of the research project by the Free State of Thuringia (Germany) and the European Union (EFRE) is highly acknowledged (FKZ: 2012 FGR 0013).

References: [1] Frosch, T.; Yan, D.; Popp, J. Anal Chem 2013, 85, 6264-6271. [2] Hartung, A.; Kobelke, J.; Schwuchow, A.; Wondraczek, K.; Bierlich, J.; Popp, J.; Frosch, T.; Schmidt, M. A. Optics Express 2014, 22, 19131. [3] Hanf, S.; Keiner, R.; Yan, D.; Popp, J.; Frosch, T. Anal Chem 2014, 86, 5278-5285.

CPP 28.5 Tue 15:00 C 264

**Analysis of vibrating microstructures using dynamic scanning electron microscopy (DySEM)** — •Maria Schröter[1], Martin Ritter[2], Matthias Holschneider[3], and Heinz Sturm[1] — [1]BAM 6.9, Federal Inst. Materials Research, Berlin — [2]Electron Microscopy, TU Hamburg-Harburg — [3]Inst. Mathematics, Univ. Potsdam

The term "DySEM" (Dynamic Scanning Electron Microscopy) denotes an experimental procedure for measuring the vibrational dynamics of a microscale oscillator using a scanning electron beam. The DySEM technique enables the direct observation of freely vibrating structures, including several modes in the normal and torsional direction as well as their higher harmonics. Additionally, the DySEM images contain characteristic amplitude-dependent image features.

Thus, this method is a tool of modal analysis of microscale structure in oscillation, which is frequently used in micro- and nanoelectromechanical systems (MEMS and NEMS) and where an optimization of the design parameters often only can be achieved by imaging the vibration (1). The advantage of DySEM technique is the ability to distinguish between artefacts based on the imaging process and features which carry relevant information (i.e. nonlinear mechanical behavior of the micro-oscillator, especially in tapping mode microscopy of soft matter). Our talk concentrates on experimental issues, the underlying theory of the experimental results is shown in a corresponding poster.

(1) Schröter; Dissertation TU Berlin (2014)

CPP 28.6 Tue 15:15 C 264

**Characterization of deformation and fracture behaviour of semi-crystalline polymers by thermography with high lateral and time resolution** — •Schneider Konrad[1] and Stein Marcus[2] — [1]Leibniz-Institut für Polymerforschung Dresden, Dresden, Germany — [2]Technische Universität Dresden, Fakultät Maschinenwesen, Institut für Verarbeitungsmaschinen und Mobile Arbeitsmaschinen, Germany

Plastic deformation during yielding and stretching as well as fracture propagation in semi-crystalline polymers dissipates a considerable amount of energy. This leads to a local temperature increase, connected with a change of local molecular mobility. By infrared thermography with high lateral and time resolution these changes can be quantified. With measurements on Poly(ethylene terephthalate) (PET) as well as Polycarbonate (PC) it will be demonstrated, how locally the glass transition temperature can be exceeded and how the deformation process in detail is affected by the really appeared temperature. Also the appearance of cavitation will be mainly affected by the thermal fields in the necking zone. Finally the strongly located energy dissipation during fracture will be presented and discussed in detail. This discussion shall throw a new light on the relevant molecular rearranging processes.

CPP 28.7 Tue 15:30 C 264

**Resolution Enhancement For Low-Temperature Scanning Microscopy By Cryostat Immersion Imaging** — •Michael Metzger[1], Alexander Konrad[1], Alfred J. Meixner[1], and Marc Brecht[2] — [1]Institute of Physical and Theoretical Chemistry, University of Tuebingen, Germany — [2]Zurich University of Applied Science, Institute of Applied Mathematics and Physics, Winterthur, Switzerland

One convenient way to increase the resolution of e.g. fluorescence images is realized by confocal microscopy with an objective of high numerical aperture and immersion oil. The combination of immersion fluids with high-performance objectives is however exceedingly problematic under low temperature conditions. A new construction of a scanning stage and a well-chosen immersion fluid enables us to immerse an objective together with the sample positioned inside a cryostat at cryogenic temperatures. Heating the sample chamber over the melting point of an appropriate chosen immersion fluid (e.g. 1-propanol) allows us to move the objective into the melted immersion droplet and thereby to increase the refractive index between the objective lens and the sample. We recorded confocal fluorescence images of quantum dots at 160 K with a high NA objective. By determining the point spread function of imaged single quantum dots the effective numerical aperture was appointed to be larger than unity (1.08). The presented method provides new opportunities e.g. for studies on biological systems like vitrified cells at low temperature and is also of relevance for correlative light and electron cryo microscopy.

CPP 28.8 Tue 15:45 C 264

**Stable Metallic Silver Nanostructures by Atomic Vapour Deposition on a Volatile Liquid Jet** — Michael McNally, Gediminas Galinis, Oliver Youle, Ruth Chantry, and •Klaus von Haeften — Department of Physics and Astronomy, University Leicester, Leicester, LE1 7RH, UK

Synthesis of nanoparticles in liquids is a diverse field covering a range of powerful empirical methods to produce a variety of shapes, structures and compounds. The majority of methods are based on chemical reduction, inherently restricting the choice of starting materials and stabilisers. We show that by using a liquid micro jet it is possible to perform physical vapour deposition directly into a high vapour pressure liquid, producing a phase of intrinsically stable metallic silver nanoparticles. Silver nanoparticles produced by deposition directly into ethanol exhibit a plasmon resonance in the optical absorption spectrum which is unchanged over more than a year, indicative of metallic behaviour and exceptionally stability, without additives. TEM imaging show evenly dispersed spherical particles with a log-normal distribution of sizes peaking at 2.5 nm. Our observations suggest that atomic silver arrives at the liquid surface, becomes trapped, nucleates and grows into nanoparticles by subsequent collisions with silver atoms and ions. The particles grow step by step, or stabilise. This process occurs within the transit time of the liquid jet of 100 ms. Our method enable the investigation of metal vapour-solvent interactions of a practically unlimited range of metal-solvent combinations, the elucidation of the role of stabilisers and the production novel nanoparticles.

## CPP 29: Reaction-Diffusion Systems (Joint session DY, CPP)

Time: Tuesday 14:30–16:15 Location: BH-N 243

CPP 29.1 Tue 14:30 BH-N 243

**Front and Turing patterns induced by Mexican-hat-like nonlocal feedback.** — •Julien Siebert and Eckehard Schöll — Technische Universität, Berlin, Deutschland

We consider the effects of a Mexican-hat-shaped nonlocal spatial coupling, i.e., symmetric long-range inhibition superimposed with short-range excitation, upon front propagation in a model of a bistable reaction-diffusion system. We show that the velocity of front propagation can be controlled up to a certain coupling strength beyond which spatially periodic patterns, such as Turing patterns or coexistence of spatially homogeneous solutions and Turing patterns, may be induced. This behaviour is investigated through a linear stability analysis of the spatially homogeneous steady states and numerical investigations of the full nonlinear equations in dependence upon the nonlocal coupling strength and the ratio of the excitatory and inhibitory coupling ranges.

CPP 29.2 Tue 14:45 BH-N 243

**Front propagation in channels with spatially modulated cross-section** — •Steffen Martens, Jakob Löber, and Harald Engel — Technische Universität Berlin, Berlin, Germany

The problem of front propagation in a three-dimensional channel with spatially varying cross-section is reduced to an equivalent reaction-diffusion-advection equation with boundary-induced advection term [S. Martens et al.,*PRE*, in press; arXiv:1406.7516]. Treating the advection term as a weak perturbation, an equation of motion for the front position is derived. We analyze channels whose cross-sections vary periodically with $L$ along the propagation direction of the front. Taking the Schlögl model as representative example, we calculate analytically the nonlinear dependence of the front velocity on the ratio $L/l$ where $l$ denotes the intrinsic front width. Our analytical results agree well with the results obtained by numerical simulations. In particular, the peculiarity of boundary-induced propagation failure for a finite range of $L/l$ values is predicted by analytical calculations. Lastly, we demonstrate that the front velocity is determined by the suppressed diffusivity of the reactants for $L \ll l$.

CPP 29.3 Tue 15:00 BH-N 243

**Kinetics of a chemical clock reaction in a microflow** — •Robert Raimund Niedl[1], Alexander Anielski[1], Igal Berenstein[2], and Carsten Beta[1] — [1]Biological Physics, Universität Potsdam, Germany — [2]Nonlinear Physical Chemistry Unit,Université libre de Bruxelles, Brussels

We study the dynamics of the autocatalytic iodate-arsenite reaction in

PDMS-based microfluidic devices under continuous flow conditions. If a critical amount of initializer is present, a color reaction is triggered by a nonlinear autocatalytic process. We investigate the kinetics of the clock depending on the various input concentrations and in different channel geometries. We could show that due to delayed mixing in the microchannel, higher local initiator concentrations occur, so that the reaction runs up to seven times faster, than in a macroscopic well-mixed volume.

CPP 29.4 Tue 15:15 BH-N 243

**Three-Dimensional Autonomous Pacemaker in Excitable Media** — •Arash Azhand, Jan F. Totz, and Harald Engel — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

In experiments with the photosensitive Belousov-Zhabotinsky reaction (PBZR) we found a stable three-dimensional organizing center that periodically emits trigger waves of chemical concentration. Our experiments are performed in a parameter regime with negative line tension using an open gel reactor to maintain stationary non-equilibrium conditions. The observed periodic wave source is formed by a scroll ring stabilized due to its interaction with a no-flux boundary.

Sufficiently far from the boundary, the scroll ring expands and undergoes the negative line tension instability before it finally develops into scroll wave turbulence. Our experimental results are reproduced by numerical integration of the modified Oregonator model for the PBZR. In the numerical simulations besides stationary also breathing self-organized pacemakers have been found where both the radius of the scroll ring and the distance of its filament plane to the no-flux boundary undergo stable limit cycle oscillations.

[1] Y. Kuramoto, Chemical Oscillations, Waves, and Turbulence (Dover Publications, 2003)

[2] M. Stich, I. Ipsen, and A.S. Mikhailov, Phys. Rev. Lett. 86, 4406 (2001)

[2] A. Azhand, J. F. Totz, and H. Engel, EPL 108, 10004 (2014)

CPP 29.5 Tue 15:30 BH-N 243

**Critical coupling and bifurcations in two-dimensional oscillator arrays undergoing the Belousov-Zhabotinsky reaction** — •Claudia Lenk and J. Michael Köhler — Institut für Chemie und Biotechnologie, TU Ilmenau, Ilmenau, Deutschland

Spatio-temporal dynamics of many biological and chemical systems depend on coupling of individual oscillators e.g. catalyst particles, the heart cells during atrial fibrillation or neuronal networks. In these systems, irregular patterns and bifurcations of frequency are most often observed in regions of critical coupling strength. To elucidate the influence of local coupling of individual oscillators we perform on one hand experiments of the Ferroin-catalyzed Belousov-Zhabotinsky reaction in silica gels and on the other hand numerical calculations of the FitzHugh-Nagumo (FHN) model, both with a catalyst distribution in form of a micro spot pattern. We observe transitions to multiple period oscillations and amplitude oscillations in dependence of spot distance and size. Furthermore, these transitions can also be observed due to gradients of the spot distance for parameter ranges, which otherwise do not show these bifurcations. The identifiation of bifurcation parameters is done in the numerical simulations. Experimental results confirm the numerical analysis.

CPP 29.6 Tue 15:45 BH-N 243

**Electrodissolution of silicon: Self-organized patterns in space and time** — •Konrad Schönleber, Lennart Schmidt, and Katharina Krischer — TU München, Deutschland

The oscillatory electrodissolution of silicon in fluoride containing electrolytes has been studied for decades. Still many basic aspects concerning this system remain unknown, most prominently the mechanism giving rise to the oscillations.

In the present work, some key features of this oscillatory mechanism will be presented. It will be secifically shown that the system seems to have a built-in memory of its current state even when perturbed drastically.

For n-doped silicon, pattern formation is observed under limited illumination. Remarkably, these patterns often consist of different dynamical states coexisting on the electrode, the most striking example of which are the so-called 'chimera states'. The pattern formation can be well understood in theory, when treating the silicon as an oscillatory medium close to the onset of oscillations. A comparison of theoretical simulations and experiments will be given.

CPP 29.7 Tue 16:00 BH-N 243

**Enhancement of dimerization in a 1D-out-of-equilibrium system** — •Philipp Seifert[1,2], Patrick Hillenbrand[2], Vladimir Palyulin[2], and Ulrich Gerland[2] — [1]Ludwig-Maximilians-Universität München, 80799 Munich, Germany — [2]Theory of Complex Biosystems, Physik-Department, Technische Universität München, James-Franck-Strasse 1, D-85748 Garching, Germany

Mutual enhancement of polymerization and accumulation was recently found to be essential for spontaneous synthesis of long polynucleotides from nucleotide monomers, which is perceived as a substantial step in the emergence of early life [1]. The major driving force behind this effect is a thermally induced drift, which increases the concentration of monomer units in a certain volume and hence enhances the subsequent polymerization. Here we study a simple model of a drift-diffusion system coupled with a reversible dimerization process. We introduce a measure of the global chemical balance, which characterizes the enhancement of dimerization relative to a homogenous system. Numerical and analytical results show a nontrivial dependence of this enhancement on the physical properties of the system. Specifically, we find that the ratio of timescales between physical and chemical processes critically influences the steady state properties.

[1] Mast, C. B., Schink, S., Gerland, U., and Braun, D. (2013). Proc. Natl. Acad. Sci. USA, 110, 8030-8035.

## CPP 30: P2: Organic Electronics and Photovoltaics

Time: Tuesday 14:00–16:00 Location: Poster B

CPP 30.1 Tue 14:00 Poster B

**NMR of $^{129}$Xe and $^{13}$C or $^{31}$P - Construction of a UHV Compatible Double Resonance Probe** — •Lars Kraft, Alexander Potzuweit, Anuschka Schaffner, and Heinz Jänsch — FB Physik, Philipps Universität Marburg, 35032 Marburg

The goal of the current project is the investigation of internal atomic layers by NMR techniques. As conventional NMR is by far not sensitive enough to address few layers of semiconductor material grown on a substrate, the sensitivity must be enhanced by 3 to 5 orders of magnitude. This can be achieved by dynamic nuclear polarization (DNP), i.e. the transfer of polarization from a hyperpolarized $^{129}$Xe film to possible probe nuclei like $^{31}$P or $^{13}$C.

Here we describe the technical development of an NMR probe simultaneously resonant to two different kinds of nuclei in an UHV environment which is necessary for DNP. The idea is to extend the existing probe by coupling a second circuit that provides the additional resonance frequency leaving the present UHV setup unchanged. The main task is to match the signal and power transmission between the probe and the spectrometer.

The DNP process is most efficient at close contact. Therefore a $^{13}$C graphene substrate may be a first material investigated. For an internal $^{31}$P layer inside a heterostructure the substrate must contain the layer within a few atomic distances from the surface.

Supported by DFG und GRK 1782.

CPP 30.2 Tue 14:00 Poster B

**Surface properties and crystallization behavior of thin films of a high mobility electron-transporting semicrystalline polymer studied with MUSIC-mode AFM** — •Mario Zerson[1], Martin Neumann[1], Dieter Neher[2], and Robert Magerle[1] — [1]Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Chemnitz, Germany — [2]Institute of Physics and Astronomy, University of Potsdam, Potsdam-Golm, Germany

We study the crystallization behavior, the surface structure, and the nanomechanical properties of the thiophene-based semiconducting copolymer P(NDI2OD-T2) using multi-set point intermittent contact (MUSIC) mode atomic force microscopy (AFM). The influence of the annealing temperature and the film thickness on the resulting morphology is studied. The crystalline lamellae form larger domains which differ in the effective tip-sample interaction, the energy dissipated between the tip and the sample, and the tip indentation into the surface. The two types of domains are attributed to the two known crystalline forms of P(NDI2OD-T2). In contrast to other semicrystalline polymers, we detect no amorphous top layer; the edges of the crystalline lamellae are exposed to the surface. The tip indentation into the surface is attributed to the thickness of the layer of side chains, which covers the edges of the crystalline lamellae. Films annealed at 320°C form terraces with a step height of 2.2 nm. The terraces are formed by the edges of closely spaced crystalline lamellae. The step height between adjacent layers correspond to the height of monomolecular layers of edge-on oriented polymer chains.

CPP 30.3 Tue 14:00 Poster B

**Interplay of Environmental and Molecular Factors in Backbone Order of a Semiconducting Polymer: A DFT Study of Polyfluorenes** — •Elizabeth Lupton[1], Feng Liu[2], and Bernhard Dick[1] — [1]Institute for Physical and Theoretical Chemistry, University of Regensburg, Universitaetsstrasse 31, 93053 Regensburg, Germany — [2]Department of Materials Science and Engineering, University of Utah, Salt Lake City, UT 84112, USA

The environmental and molecular parameters which determine the nature of chromophores in polymeric systems are identified through systematic studies of molecules with well defined structures. Polyfluorenes exhibit both disordered and ordered phases which depend on the degree of planarity of the conjugated polymer backbone and can be distinguished spectroscopically. We examine the intrinsic and extrinsic factors that determine the ordering of the backbone using DFT and TDDFT calculations. We determine that a stable ordered phase with a specific torsional angle between repeat units exists which planarizes on exitation, and that specific deviations from the ordering, such as rotations which cause deviations from backbone linearity, do not affect the molecules' ability to planarize. The results demonstrate the complicated interplay between external confinement, intermolecular properties and photoexcitation in determining the structure and photophysics of organic semiconducting polymers.

CPP 30.4 Tue 14:00 Poster B

**Morphological and dynamic ordering of the semiconducting polymer PBTTT** — Matthias J. N. Junk[1], Dmytro Dudenko[2], Nichole Cates Miller[3], Sean Sweetnam[3], Michael D. McGehee[3], Bradley F. Chmelka[1], Michael R. Hansen[2,4], Kurt Kremer[2], •Anton Melnyk[2], and Denis Andrienko[2] — [1]University of California, Santa Barbara, California 93106, U.S.A. — [2]Max-Planck-Institute für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany — [3]Stanford University, Stanford, California, 94305, U.S.A. — [4]Aarhus University, Gustav Wieds Vej 14, DK-8000 Aarhus C, Denmark

Molecular dynamics of the conjugated polymer poly(2,5-bis(3-hexadecylthiophen-2-yl)thieno[3,2-b]thiophene) (PBTTT-C16) are quantitatively measured using solid-state NMR spectroscopy and compared to atomistic molecular dynamics simulations. The comparison reveals crystalline domains that have well-ordered interdigitated alkyl sidechains with restricted rotational mobilities up to the terminal methyl group, accompanied by well-ordered polymer backbones. Amorphous domains, which comprise 50% of as-synthesized PBTTT-C16, consist of disordered side chains with a significantly higher degree of rotational mobility. from planarity in amorphous domains. In conjunction with a decreased $\pi-\pi$ stacking order, the partially interrupted backbone conjugation may be predominantly responsible for significantly decreased charge-carrier mobility in the amorphous regions.

CPP 30.5 Tue 14:00 Poster B

**The effect of crystallization on the charge mobility through P3HT-PC70BM films** — •Kaiwan Jahanshahi[1], Vladimir Dyakonov[1,2], and Carsten Deibel[3] — [1]Experimental Physics VI, Julius-Maximilian University of Würzburg, 97074 Würzburg, Germany — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg, Germany — [3]Institut für Physik Optik und Photonik kondensierter Materie, Technische Universität Chemnitz, 09107 Chemnitz, Germany

Poly(3-hexylthiophene) (P3HT) and fullerene (PC70BM) mixtures are one of the most important semiconducting polymer-fullerene blend materials in organic photovoltaic. Because of the intricacy of the crystal formation in these type of polymer-fullerene blends, the relationship between their crystalline structure and mobility of the charges through their bulk structure is not comprehensively discussed. In this study we have used a well controlled process of solvent annealing technique in order to grow well-ordered P3HT-PC70BM spherulites as an active layer in our solar cells which enabled us to employ time of flight (TOF) and OTRACE techniques to measure the mobility of the charges through the bulk of the crystalline film and perpendicular to the plane of the spherulitic crystals and compare them to the mobility of the charges through an amorphous active layer.

CPP 30.6 Tue 14:00 Poster B

**Hot charges speed up non geminate recombination but have no effect on device performance** — •Jona Kurpiers, Steve Albrecht, and Dieter Neher — Institute of Physics and Astronomy, Soft Matter Physics, University of Potsdam, D-14476 Potsdam

In this work, we use time delayed collection field (TDCF) experiments with exceptionally high time resolution to investigate the charge carrier dynamics in the PCDTBT:PC70BM system. Although this system has a high fill factor of around 70% and an internal quantum efficiency approaching unity under steady state illumination conditions, TDCF experiments reveals non-geminate recombination on the 10 ns time-scale, even for charge carrier densities comparable to one sun illumination. This loss becomes significantly accelerated at higher pulse fluence. To identify the reason for this rapid loss, the recombination dynamics was further investigated with constant white light background illumination, which introduces a tunable steady state carrier density, and on thicker devices. We observe that the short term decay dynamics is not affected by the background carrier density. It is concluded that the main reason for the nongeminate loss observed at the 10 ns time scale is recombination of hot charges close to the contacts. As recombination occurs mainly between hot electrons and holes, this loss channel seems to be insignificant under steady state illumination. Our result imply that transient experiments, considering the dynamics of *freshly-generated* charges should be considered with great care when aiming at the understanding of device function under steady-state illumination conditions.

CPP 30.7 Tue 14:00 Poster B

**Calculation of excited states in donor-acceptor heterojunctions via GW-BSE/MM** — •Jens Wehner, Denis Andrienko, and Björn Baumeier — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Modelling charge separation in organic solar cells must take into account the quantum nature of the photo-induced excitations and the influence of large-scale morphological order to fully understand and predict the properties of the dominant processes. This requires multiscale methods to capture the quantum mechanics of the problem while keeping the computational cost tractable.

Here, we use a QM/MM approach based on GW-BSE and polarizable force-fields to study the conversion of Frenkel excitons into charge transfer states at prototypical small-molecule C60 donor-acceptor interface. The iterative self-consistent solution of the coupled GW-BSE/MM problem allows us to analyze the influence of the molecular alignment and the long-range order at the interface on the driving force behind the charge separation process.

CPP 30.8 Tue 14:00 Poster B

**Charge Transfer Between Single-Wall Carbon Nanotubes, Fullerenes and Polymers** — •Michael Auth[1], Andreas Sperlich[1], Florian Späth[3], Tobias Hertel[3], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg — [2]ZAE Bayern, 97074 Würzburg — [3]Physical and Theoretical Chemistry II, Julius Maxim- ilian University of Würzburg

Single-Wall Carbon Nanotubes (SWNT) are of interest to improve the spectral response of organic photovoltaic cells (OPV) due to their near-infrared absorption bands. Additionally, their unique electrical properties, stemming from their one-dimensionality, recommend them to improve charge transport properties of electrons and holes in existing OPV systems. However, it is to date unclear, whether SWNTs act as electron donors or acceptors in conjunction with common OPV materials. Before we can optimize those systems, we need to understand how the SWNTs contribute to charge transfer processes. In this study semiconducting (6,5) SWNTs are combined with widely known OPV materials, such as the fullerene acceptor $PC_{60}BM$ and the polymer P3HT. Using Electron Paramagnetic Resonance (EPR) we can distinguish charge carriers residing on different conjugated organic molecules and SWNTs. We found specific EPR signatures for charges located on either SWNT, P3HT or $PC_{60}BM$. Our measurements hint at the potential ambipolarity of SWNTs, leading to either hole transfer from $PC_{60}BM$ or electron transfer from P3HT.

CPP 30.9 Tue 14:00 Poster B

**Determination of the CT energy of organic small molecule solar cells by different methods** — •Theresa Linderl, Mark Gruber, Stefan Grob, Ulrich Hörmann, Alexander Hofmann, and Wolfgang Brütting — Universität Augsburg, 86135 Augsburg, Germany

The open-circuit voltage $V_{OC}$ of organic solar cells is limited by the formation of a charge transfer (CT) state at the donor-acceptor interface. We determine the energy of the CT state for small molecule organic solar cells by different methods and compare the obtained values. Electroluminescence (EL) spectroscopy on heterojunction devices together with the spectra of single layer devices of the individual materials are used to determine the CT feature in the spectrum. For voltages just above $V_{OC}$ an additional feature can be detected in the low energy range that cannot be attributed to any of the individual materials. Together with sensitive IPCE (Incident Photon to Current Efficiency) measurements the CT energy can be determined and compared to the values derived from temperature dependent measurements of the current-voltage ($j$-$V$) characteristics. Both, dark and illuminated $j$-$V$ curves can be used to determine the CT gap energy. We find that the energy loss from the CT energy to $q \cdot V_{OC}$ at room temperature is 0.55 eV for all investigated material systems.

CPP 30.10 Tue 14:00 Poster B

**Comparison of DFT functionals and insights into photo-induced charge separation in Ruthenium terpyridine complexes** — •Julia Preiss[1,2], Benjamin Dietzek[1,3], Todd Martínez[2,4], and Martin Presselt[1,4] — [1]Institute for Physical Chemistry and Abbe Center of Photonics, Friedrich-Schiller-University Jena — [2]SLAC National Accelerator Laboratory, Menlo Park, California 94309, USA — [3]Leibniz Institute of Photonic Technology (IPHT) Jena — [4]Department of Chemistry and PULSE Institute, Stanford University

Ruthenium polypyridine-type complexes are an extensively used sensitizer to convert solar energy into chemical and/or electrical energy, and can be tailored via their metal-to-ligand-charge transfer (MLCT) properties. We explore the nature of the $^1$MLCT states of remotely substituted Ru(II) model complexes by both experimental and theoretical techniques. Two model complexes with electron-withdrawing (-$NO_2$) and electron-releasing (-$NH_2$) groups were synthesized, including a phenylene spacer to serve as spectroscopic handle and to confirm the contribution of the remote substituent to the $^1$MLCT transition. The $[Ru(tpy)_2]^{2+}$-based complexes (tpy is tpy 2,2':6',2"-terpyridine) are further de-symmetrized by tert-butyl groups to yield uni-directional $^1$MLCTs with large transition dipole moments, beneficial for related directional charge transfer processes. Detailed comparison of experimental spectra with theoretical calculations based on density functional theory, revealed different properties of the optically active bright $^1$MLCT state already at the Franck-Condon point.

CPP 30.11 Tue 14:00 Poster B

**Performance P3HT:PCBM solar cells modified with iron oxide nanoparticles** — •Daniel Moseguí González[1], Volker Körstgens[1], Yuan Yao[1], Lin Song[1], Gonzalo Santoro[2], Stephan Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748, Garching — [2]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607, Hamburg

Among the different systems studied in organic solar cells, the combination of P3HT:PCBM has received the highest attention due to easy commercial availability. However, regarding further boost in efficiencies, doping with heavy metals has shown interesting behavior. The presence of heavy metals increases the L-S coupling in the system, increasing the rate of intersystem crossing, and thereby lowering the averaged recombination rate. 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 advanced scattering techniques. Spectral behavior and electrical response of devices are also investigated, providing altogether a detailed picture of doped systems.

CPP 30.12 Tue 14:00 Poster B

**Characterization and comparison of the optical properties of high-efficiency polymers PBDTT-FTTE and PBT7** — •Franziska Löhrer, Shuai Guo, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Organic photovoltaics are gaining impact as a feasible alternative to conventional silicon solar cells. Using polymers as active material has several potential advantages, for instance reduced production costs and an increased device flexibility. A prominent and well-understood example is P3HT, which has been diligently investigated in the last years. However, efficiencies stay far below those of competing inorganic solar cells. Recent research efforts focus on identifying new high-efficiency polymers in order to enhance the cell performance. This has led to the development of high-efficiency materials such as PTB7 or the new PBDTT-FTTE with reported efficiencies approaching 10 %. However, these materials are still very cost-intensive and their functionality is not yet fully understood. Previous morphological investigations linked to the device performance give first insights into the working mechanisms of PTB7 based solar cells. In the present study we investigate the optical and morphological properties of PBDTT-FTTE in comparison to those of PTB7 and the well-known P3HT. Applied characterization techniques include UV/Vis- and IV-measurements, optical microscopy, AFM, as well as XRR and GISAXS/GIWAXS. Exploratory solar cells link the conversion efficiency to parameters such as the composition and morphology of the active layer.

CPP 30.13 Tue 14:00 Poster B

**Resonant GISAXS of conducting polymers** — •Mihael Coric[1], Nitin Saxena[2], Jan Wernecke[3], Stefanie Langner[3], Peter Müller-Buschbaum[2], Michael Krumrey[3], and Eva M. Herzig[1] — [1]Technische Universität München, Munich School of Engineering, 85748 Garching, Germany — [2]Technische Universität München, LS Funktionelle Materialien, 85748 Garching, Germany — [3]Helmholtz-Zentrum Berlin BESSY, Physikalisch-Technische Bundesanstalt (PTB),Albert-Einstein-Straße 15, 12489 Berlin

In the last few years the use of X-ray for investigation of morphological structure of polymeric thin films in photovoltaic has increased. It is a suitable method to investigate morphological changes in the polymer film. So far mostly hard x-ray around 10 keV are used to probe the samples. The disadvantage of using hard x-rays when looking at polymers is that the scattering contrast is low and therefore they are difficult to distinguish from each other.

Another approach that is pursued in this work is choosing x-ray energies that are near absorption edges of certain elements. Using x-rays at absorption edges enables a much higher contrast between the different materials, increasing the distinguishability of the different components within the active film of the organic solar cell. In combination with grazing incident small angle scattering (GISAXS), the use of resonant x-rays at the absorption edge, offers a sophisticated way to investigate morphological changes of the polymer blend, making it a promising method for future use.

CPP 30.14 Tue 14:00 Poster B

**Characterization of PTB7-Th:PC71BM bulk heterojunction solar cells** — •Edoardo Barabino, Weijia Wang, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Organic photovoltaic devices are approaching the efficiency of traditional silicon based solar cells and are promising low-cost and ease production via roll-to-roll printing. In the bulk heterojunction morphology a low-band gap conjugated polymer (electron donor) and a fullerene derivative (acceptor) are blended together. The low-band gap polymer brings to the production of more excitons due to absorbing more photons (higher short circuit current) and to higher open circuit voltage. Recently a novel PTB7 derivative, denoted as PTB7-Th, has shown efficiency values close to 10%. We investigate organic solar cells made by this polymer PTB7-Th and PC71BM current-voltage characterization. In addition external quantum efficiency (EQE), UV-Vis absorption and photoluminescence spectroscopy are applied to further characterize there solar cells. Additionally the active layer surface structure is inspected via atomic force microscope (AFM).

CPP 30.15 Tue 14:00 Poster B

**Evolution of the Morphology during Functional Stacks Build-up of P3HT:PCBM Inverted Solar Cells** — •Weijia Wang[1], Stephan Pröller[1,2], Martin A. Niedermeier[1], Volker Körstgens[1], Martine Philipp[1], Bo Su[1], Shun Yu[3,4], Stephan V. Roth[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-

Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]Technische Universität München, MSE, Herzig Group, Lichtenbergstr. 4, 85748 Garching — [3]DESY, Notkestraße 85, 22603 Hamburg — [4]KTH, School of Chemical Science and Engineering, Teknikringen 56-58, 100 44 Stockholm, Sweden

Poly(3-hexylthiophene-2,5-diyl) (P3HT):phenyl-C61-butyric acid methyl ester (PCBM) bulk heterojunction (BHJ) is a well established model system for organic solar cells. Introducing an inverted geometry in a BHJ solar cell has been applied in several groups to achieve stable and more efficient solar cells. However, the basic understanding of the evolution of the morphologies during the complex functional stack assembling is still unknown. Therefore, the gradual evolution of the P3HT:PCBM morphology is investigated by AFM and GISAXS measurements. The inverted P3HT:PCBM BHJ solar cell show an increased power conversion efficiency as compared to the standard geometry, which is explained by the different morphology of the active layer.

CPP 30.16 Tue 14:00 Poster B

**Morphology of PCPDTBT:PC71BM Thin Films for Organic Photovoltaics** — •Christoph J. Schaffer[1], Johannes Schlipf[1], Bo Su[1], Efi Dwi Indari[1], Sigrid Bernstorff[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Deptartment, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]Elettra Sincrotrone Trieste, 34012 Basovizza, Italy

As a convenient pathway to ever more efficient polymer-based solar cells, the use of solvent additives has proven to boost the power conversion efficiencies of several low-bandgap polymer:fullerene systems. The strong improvement of solar cell characteristics is thereby mostly related to a drastic change in nano morphology of the active blend layers induced by the use of solvent additives. It is, however, not yet fully understood how the use of certain solvent additives influences the morphology and the stability of the specific blend layers.

In this work, we investigate the morphological changes of PCPDTBT:PC71BM films induced by the use of 1,8-octanedithiol by means of grazing incidence small and wide angle x-ray scattering and X-ray reflectivity and find that ODT enhances micro phase separation and consequently polymer crystallization. The findings are complemented by UV/Vis and photoluminescence spectroscopy. Furthermore, we show that the optical characteristics of blend films with ODT are highly unstable on a timescale of days.

CPP 30.17 Tue 14:00 Poster B

**Morphology tuning and interface engineering of new donor model layers** — Felix Herrmann[1], Rainer Beckert[2], Benjamin Dietzek[1,3], and •Martin Presselt[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, D-07743 Jena, Germany — [2]Institute of Organic Chemistry and Macromolecular Chemistry, Friedrich Schiller University Jena, D-07743 Jena, Germany — [3]Leibniz Institute of Photonic Technology (IPHT), Albert-Einstein-Str. 9, 07745 Jena, Germany

In the last years the efficiency of organic solar cells has been greatly enhanced towards actually 12%. These enhancements were mainly driven by using and synthesizing new active materials. The basic processes of exciton dissociation and recombination at the donor-acceptor interface are extensively debated because in bulk heterojunction devices capturing the nature of the interface and its morphology is challenging. Using the Langmuir-Blodgett technique allows for the production of donor- acceptor bilayer structures with defined interfaces and tunable ordering as model systems. We focus on tuning of the morphology of individual layers composed of merocyanines of varied chromophore size and their optical properties. Thus, one essential precondition for the investigation of defined donor-acceptor interfaces is accomplished.

CPP 30.18 Tue 14:00 Poster B

**degradation in printed polymer:fullerene thin films for organic photovoltaics** — •Jan Richard Stockhausen, Peter Müller-Buschbaum, and Christoph Schaffer — TU München, Physik-Department, LS Funktionelle Materialien, James Franck-Str. 1, 85748 Garching, Germany

In comparison to conventional silicon solar cells, organic photovoltaics (OPVs) offer several advantages, like ease of production and a high versatility. Nevertheless, their lifetime needs to be prolonged, so that a profitable large-scale production becomes feasible. Therefore, a detailed understanding of the degradation mechanisms is necessary. In the present investigation, we address UV induced aging of PCPDTBT:PC71BM and P3HT:PCBM active layers, printed in a positive shim mask slot dye coater. Changes in the films due to accelerated aging are investigated by means of atomic force microscopy (AFM), X-ray reflectivity (XRR) and UV/Visible light spectroscopy (UV/Vis).

CPP 30.19 Tue 14:00 Poster B

**Exploring the impact of inter-segmental mixing and photodegradation on the photovoltaic performance of donor-acceptor-type polymer solar cells using a novel particle-based multiscale solar-cell algorithm** — Anton Pershin, Sergii Donets, and •Stephan Baeurle — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, 93040 Regensburg

Polymer solar cells possess a promising perspective for generating renewable energy at affordable costs, provided their performance and durability can be improved considerably. To this end, several experimental techniques have been devised recently, establishing a direct link between the local morphology, local opto-electronic properties and device performance. However, their reliability is still unclear to this day. Here, we demonstrate by using a novel particle-based multiscale solar-cell approach [1] and comparing its results with the ones of a field-based solar-cell algorithm that inter-mixing of the electron-donor(D)- and -acceptor(A)-type of segments in a lamellar-like PFB-F8BT blend causes that the major part of the charge generation and charge transport takes place in the bulk of the nanophases of the nanostructured polymer solar cells in agreement with recent experimental measurements and not, as commonly believed, at the visible domain boundaries of the DA interface. Moreover, we demonstrate that photo-oxidation of the fluorene moiety of the F8BT phase leads to keto-induced electron trapping, resulting in a deteriorated electronic transport efficiency in photodegradated PFB-F8BT-blend devices. Literature: [1] A. Pershin, S. Donets, S.A. Baeurle, Polymer 55, 3736 (2014).

## CPP 31: P3: Hybrid Photovoltaics and Preovskites

Time: Tuesday 14:00–16:00 Location: Poster B

CPP 31.1 Tue 14:00 Poster B

**Influence of the Solvent on the Charge Transport Dynamics in *ZnO*-based Dye-Sensitized Solar Cells** — •Christoph Richter, Max Beu, and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Heinrich-Buff-Ring 16, D-35392 Giessen

In electrodeposited *ZnO*-based dye-sensitized solar cells (DSCs) the common solvent is a mixture of 4:1 vol % ethylene carbonate : acetonitrile. Since ethylene carbonate is a solvent with a high viscosity compared to acetonitrile non-negligible contributions to the series resistance were observed. To overcome this problem we have studied different mixtures of 3-methoxypropionitrile, valeronitrile or ethylene carbonate with acetonitrile. A detailed photoelectrochemical analysis was conducted to understand the differences observed in the measured IV-curves. By using intensity modulated current and photovoltage spectroscopy (IMPS, IMVS) and impedance spectroscopy (EIS) the influence of the solvent mixtures on the charge transport and recombination reactions in the DSCs could be clarified. The results, further, provide additional input to an ongoing discussion why *ZnO*-based DSCs generally lack behind the reported efficiencies of $TiO_2$-based DSCs.

CPP 31.2 Tue 14:00 Poster B

**Light harvesting structured titania films prepared by PDMS molds** — •Bo Su, Yichuan Rui, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Due to the high surface to volume ratio and the bicontinuous morphology, foam-like nanostructures are becoming more interesting in photovoltaics. To improve the power conversion efficiency, a light-trapping strategy is widely used in dye-sensitized solar cells (DSSCs) and organic photovoltaics (OPVs). In our study, we demonstrate foam-like structured titania films, which are made by blade coating and soft-molding methods, with an additional superstructure in the micrometer range. The master to implement the superstructure is prepared by photolithography. Then replica molds are made from the master with poly(dimethyl siloxane) (PDMS). Finally, the different light trapping structured titania films are prepared by applying these PDMS molds. After the fabrication of DSSCs, the photocurrent-voltage characteristics of the DSSCs are measured. The morphology of the films is characterized with SEM and AFM. The optical properties are determined by UV/Vis spectroscopy.

CPP 31.3 Tue 14:00 Poster B

**Investigation on morphology and optical properties of hybrid perovskites prepared on different substrates** — •Amrita Mandal Bera, Dan Ralf Wargulski, Ibrahim Simsek, Sergiu Levcenco, and Thomas Unold — Helmholtz-Zentrum Berlin für Materialien und Energie

Hybrid organometal perovskites have emerged as promising solar absorber material and have exhibited solar cell efficiencies more than 19% to date. The morphology of the perovskite layer is one of the most important parameters which affect solar cell efficiency. CH3NH3PbI3 has been synthesized by the two step method by converting a PbI2 layer into perovskite by immersion in methylammoniumiodide. The perovskite films prepared on different substrates [glass, fluorine doped tin oxide (FTO), FTO with TiO2 blocking layer] have been characterized by x-ray diffraction, scanning electron microscopy and optical microscope imaging. The film morphology depends on substrate type as well as processing parameters (e.g. spinning speed, deposition time and temperature). The processing parameters have been optimized to get good surface coverage. The optical properties have been investigated by measuring absorption and photoluminescence spectra at room temperature. Despite large changes in morphology of the samples they generally exhibit a strong photoluminescence band centered around 1.6 eV.

CPP 31.4 Tue 14:00 Poster B

**Investigating the morphology of $CH_3NH_3PbI_{3-x}Cl_x$ highly efficient planar perovskite solar cells** — •Johannes Schlipf[1], Lukas Oesinghaus[1], Pablo Docampo[2], Thomas Bein[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Graching — [2]LMU München, Department Chemie, Butenandtstr. 11, 81377 München

Organo-metal halide perovskites mark a paradigm shift in photovoltaic research. Recently reported power conversion efficiencies exceeding 15% are possible due to their highly crystalline nature even when processed from solution. However, film morphology is directly connected to the preparation routine and material properties like charge diffusion lengths that are intrinsically linked to photovoltaic performance. We prepare highly efficient planar methylammonium (MA) lead iodide perovskite solar cells via a two-step solution-conversion process, i.e. dipping of a previously deposited $PbI_2$ thin film into a MA-containing solution [1]. We complement electronic and optical characterization using UV-Vis spectroscopy, EQE and IV measurements with grazing incidence small and wide angle X-ray scattering (GISAXS and GIWAXS). Thereby it is possible to understand the role of film morphology and influence of film properties on solar cell performance. [1] P. Docampo, et al., Adv. Energy Mater, 4, 1400355, 2014

CPP 31.5 Tue 14:00 Poster B

**Electrical atomic force microscopy on perovskite films** — •Ilka M. Hermes, Victor W. Bergmann, Simon A. Bretschneider, Frédéric Laquai, Rüdiger Berger, and Stefan A.L. Weber — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Organolead trihalide perovskite solar cells have reached power conversion efficiencies (PCE) of more than 20%, yet not enough is known about the physics within the perovskite layer. Unusual effects have been reported, such as strong hysteretic behavior in the photocurrent-voltage curves of the cells. It remains unclear how this effect is related to the high PCE and if mechanisms like ferroelectricity or the accumulation of trapped charges cause the hysteresis. One way to tackle these questions is to investigate the nanoscale function of perovskite films, e.g. by atomic force microscopy in working devices [1].

In this work, the electronic and electromechanical properties of perovskite films were studied on nanometer scale with electrical atomic force microscopy methods. With piezoresponse force microscopy (PFM), the local piezoelectric response was visualized, providing information on possible ferroelectric domains within the film. Conductive atomic force microscopy (CAFM) was used to measure the local photocurrent. With Kelvin probe force microscopy (KPFM) contact potential variations and light-induced potential changes could be locally resolved. These experiments help to improve the understanding of the working principles of perovskite solar cells.

[1] Bergmann, V.W. et al (2014); Nature Comm. 5, 5001

CPP 31.6 Tue 14:00 Poster B

**Novel approaches for tuning optical and electronic properties of perovskites and their application in hybrid thin film solar cells** — •Lukas Oesinghaus, Johannes Schlipf, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Recently, Docampo et al. reported achieving an efficiency of up to 15.4% for solution processed planar heterojunction perovskite solar cells by using a simple two-step sequential deposition process [1].

We use a similar method, where a PbI2 film is spin cast and subsequently converted to perovskite in a mixed solution of methylammonium iodide (MAI) and methylammonium chloride (MACl), which results in a better film homogeneity as compared to single-step solution deposition and larger diffusion lengths as compared to films prepared with pure MAI solutions. Thus the overall photovoltaic performance is increased. We tune the morphology and the properties of the interfaces adjacent to the charge selective electrodes. This has an effect on the photovoltaic performance, which is characterized by UV-Vis, IV and EQE measurements. With AFM and SEM complementary structure information is achieved.

[1] Docampo et al., Adv. Energy Mater., 2014, 4, 1400355.

CPP 31.7 Tue 14:00 Poster B

**Lifetime of photogenerated charge carriers in methylammonium lead halide perovskite solar cells studied by transient photovoltage/photocurrent** — •David Kiermasch[1], Stefan Väth[1], Andreas Baumann[2], and Vladimir Dyakonov[1,2] — [1]Experimentelle Physik 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg — [2]Bayerisches Zentrum für Angewandte Energieforschung, 97074 Würzburg

In the last few years solar cells based on organo-metal halide perovskites attracted a lot of attention. Since the first publication of a solar cell with a perovskite absorber in 2009, the efficiency nowadays reaches up to 20 %. Despite that, there is a lack of understanding on the working principles in this new kind of solar cells, like the transport and the recombination of the photogenerated charge carriers. We prepared methylammonium lead halide perovskite solar cells, namely $CH_3NH_3PbI_3$ and $CH_3NH_3PbI_{3-x}Cl_x$ in a planar configuration. The lifetime and the concentration of photogenerated charge carriers are studied by transient photovoltage/photocurrent and charge extraction experiments. We discuss our results for different device configurations.

CPP 31.8 Tue 14:00 Poster B

**Recombination Dynamics in Perovskite Solar Cells probed by Time-Delayed-Collection-Field (TDCF) Experiments** — •Andreas Paulke[1], Samuel D. Stranks[2], Henry J. Snaith[2], Dieter Neher[1], and Thomas J.K. Brenner[1] — [1]Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str.24-25, D-14476 Potsdam-Golm, Germany — [2]Department of Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford OX1 3PU, United Kingdom

Time-Delayed-Collection-Field (TDCF) experiments are applied to working perovskite ($CH_3NH_3PbI_{3-x}Cl_x$) solar cells with different device architectures. In TDCF, charges generated by a nanosecond optical pulse are extracted by a large reverse voltage pulse. Thereby, the delay between the photoexcitation and the extraction is tuned over a wide range, with a minimal delay of 10ns. This allows to probe the temporal evolution of the photogenerated charges and quantify nongeminate recombination losses in the device. For comparison, the charge carrier dynamics of an all-organic device (PTB7:PC71BM) with similar performance is studied under comparable illumination conditions. We find that the predominant recombination mechanism in perovskite solar cells is very different from that of the organic cell. In particular, while the charge carrier dynamics in the all-organic cell can be described by purely bimolecular recombination with a time and fluence independent BMR coefficient, the dynamics in mesoporous-

$TiO_2$/Perovskite/Spiro and planar PEDOT:PSS/Perovskite/PCBM devices is characterized by a slow-down of the recombination rate over several microseconds.

# CPP 32: P4: Computational Physics of Soft Matter

Time: Tuesday 14:00–16:00 Location: Poster B

CPP 32.1 Tue 14:00 Poster B

**New insights into the structure of poly(p-phenylene terephthalamide: a first principles study** — •Pegah Zolfaghari[1], Ole Braukamann[1], Arno P M Kentgens[1], Robert A de Groot[1,2], and Gilles A de Wijs[1] — [1]Radboud university Nijmegen, Electronic Structure of Materials,Institute for Molecules and Materials, Netherlands — [2]Rijksuniversiteit Groningen, Solid State Materials for Electronics,Zernike Institute for Advanced Materials, Netherlands

The aromatic polyamids are a major class of polymers in recet years.This class of polyamids are of practical interest due to their high tensile strength, high elastic modulus, low elongation at breakage, and higher thermomechanical stability among other kinds of polyamids.

One of the interesting member of this class of fibres called poly, *p*-phenylene terepthalamide (hereafter PPTA). PPTA is a polymer which crystalizes in the form of 2D hydrogen-bonded sheets. It has enormous commerical applications, as already mentioned, and is sold under the commercial names of Kevlar and Twaron. The packing of the hydrogen-bonded sheets and phenyl group give rise to three different PPTA structures, including Northolt, Liu and Pb.

The calculations reveal that different PPTA structures which all exhibit herringbone packing of the phenyl groups between neighboring sheets, have similar stabilities. Also, The use of solid-state NMR experiments combined with Density Functional Theory (DFT) based calculations allows unambiguous assignment of all proton and carbon resonances of PPTA structures.

CPP 32.2 Tue 14:00 Poster B

**Water Dynamics in Aqueous TMAO Solutions: a DFT-MD Study** — •Kota Usui[1], Marialore Sulpizi[2], Johannes Hunger[1], Mischa Bonn[1], and Yuki Nagata[1] — [1]Max-Planck Institute for Polymer Research, Mainz, Germany — [2]Johannes Gutenberg University Mainz, Mainz, Germany

Trimethylamine N-oxide (TMAO) is one of the most effective agents to stabilize proteins. It has been found that TMAO is excluded from the protein's surface, which indicates that stabilization occurs via interaction of TMAO with the solvent, i.e. water. We investigate the mechanism behind the interaction of TMAO with water using DFT and force field molecular dynamics (MD) simulations. Our DFT-MD simulation reproduces the experimentally observed ~200 cm-1 red-shift of the O-D stretch vibrational peak, in contrast to force field MD. The water reorientational motion, reflected by the anisotropy decay, is significantly retarded in the vicinity of the hydrophilic O atom of TMAO (OTMAO) for our DFT-MD simulations, which is not observed in force field MD simulations. This slow-down of the anisotropy decay is found not only for the O-D group bound to OTMAO but also for the other O-D group of the same D2O molecule. Sequentially, we elucidated why force field MD predicts significantly different dynamics from the DFT-MD. To this end, we selectively calculated the anisotropy decay of those O-D groups which remain hydrogen bonded to OTMAO, which reveals the same time scale of the anisotropy decay of TMAO, indicating that the TMAO-bound D2O loses its reorientational information by following the TMAO rotational motion.

CPP 32.3 Tue 14:00 Poster B

**Electrode models for ionic liquid based capacitors** — •Kai Szuttor, Konrad Breitsprecher, and Christian Holm — Institute for Computational Physics, Stuttgart, Germany

We compare different simulation models for ionic liquid based capacitors concerning the electrode model. Therefore molecular dynamics simulations of an explicit graphite model are compared to a plain wall electrode with adapted interaction parameters. Further we compare two simulation approaches with constant potential boundary conditions to constant charged electrodes and the influence of these different methods with regard to the differential capacitance and the layering behavior of the ionic liquid at the electrode.

CPP 32.4 Tue 14:00 Poster B

**Structure and Dynamics of a Mixture of Ethylene Glycol and Water in Confinement** — •Rebecca Schmitz and Michael Vogel — Institut für Festkörperphysik, TU Darmstadt, Germany

In numerous biological processes and technical applications the motion of molecules in aqueous solutions is restricted by boundary surfaces. Therefore it is crucial to understand the impact of nanoscale confinement on structure and dynamics of liquids. We study the behavior of a mixture of ethylene glycol and water in cylindrical silica nanopores using molecular dynamics simulations. The usage of both amorphous and crystalline nanopores provides us with further insights into the role played by the structure of the confinement. For all systems we find a considerable slowdown of the structural relaxation approaching the wall while the dynamics of the inner layer is comparable to bulk behavior. But while the dynamics of the liquid is similar in all pores, its structure depends strongly on the exact configuration of the confinement. The investigation of the liquid's density profile indicates a local microphase separation induced by the confinement as one molecular species preferentially attaches to the wall. Though reported by various groups, the physics behind this effect is not very clear yet and there is no agreement on whether water or alcohol constitutes the outer layer [1,2]. As we find a very different structure of the liquid in the amorphous and the crystalline pore, our simulation study reveals further information on the influence of various parameters of the confinement.

[1] Guo et al.; J. Phys. Chem. B 118, 34 (2014)

[2] Elamin et al.; PCCP 15, 42 (2013)

CPP 32.5 Tue 14:00 Poster B

**Molecular dynamics simulation of sulfonated dimers in DMSO-Water mixtures** — •anand narayanan krishnamoorthy[1], jens smiatek[2], and christian holm[3] — [1]Institute for Computational Physics,University of Stuttgart — [2]Institute for Computational Physics,University of Stuttgart — [3]Institute for Computational Physics,University of Stuttgart

Using molecular dynamics simulations, we studied the counter ion condensation behavior of dimers with lithium ions under various mole fraction of DMSO-Water mixtures. The ionic condensation behavior show non ideal behavior for specific mole fractions of DMSO-Water mixtures. Previous study show that the non ideality of the binary mixture solution is due to the cluster formation of DMSO and Water molecules through hydorgen bonds between donor DMSO oxygen atom and hydrogen atom of Water. The non-ideal behavior, we observe can be related to solvent-solvent interactions and a preferential solvation mechanism for the dimer and the counter ions. The diffusion behavior of the binary mixture was also studied and is in good agreement with the experimental observations.

CPP 32.6 Tue 14:00 Poster B

**Unravelling the conformations of di-(perylene bisimide acrylate) by molecular modelling and free energy calculations** — Florian Spreitler[1], Michael Sommer[2,4], •Manuel Hollfelder[3], Mukundan Thelakkat[2], Stephan Gekle[3], and Jürgen Köhler[1] — [1]Experimental Physics IV and BIMF, University of Bayreuth, D-95440 Bayreuth, Germany — [2]Applied Functional Polymers, Department of Macromolecular Chemistry I, University of Bayreuth, D-95440 Bayreuth, Germany — [3]Biofluid Simulation and Modeling, Physics Department, University of Bayreuth, D-95440 Bayreuth, Germany — [4]Current address: Michael Sommer, Institute for Macromolecular Chemistry, Albert-Ludwigs-Universität Freiburg, 79104 Freiburg, Germany

We compare the results of Molecular Dynamics modelling and Umbrella Sampling on perylene bisimide acrylate dimers to the results from time-resolved fluorescence anisotropy experiments [F. Spreitler et al., Phys. Chem. Chem. Phys., 2014,16, 25959-25968]. It allows us to connect the experimentally found spectral signatures of three different fluorescence states with one non-stacked and two stacked (parallel and anti-parallel) molecular conformations. The experimental data can be reproduced for the parallel stacked conformation using a model of structural relaxation in the electronically excited state of the stacked aggregate. For the non stacked conformation agreement between experiment and modelling is only found if fast hopping of the electronic excitation (Förster energy transfer) between the perylene bisimide subunits is taken into account.

CPP 32.7 Tue 14:00 Poster B

**Ewald summation on GPU** — •Sascha Ehrhardt and Axel Arnold — Institute for Computational Physics, Stuttgart, Germany

We implemented the Ewald summation algorithm for the computation of electrostatic energies in molecular dynamics simulations for graphic cards (GPUs) using CUDA. Our implementation is part of the open source molecular dynamics package ESPResSo (http://espressomd.org).

The Ewald summation splits up the Coulomb energy sum in two sums, where one is calculated in real space and the other in reciprocal space. Because the two sums can be computed independently of each other, the real space part will be computed on the CPU using the efficient short range routines of ESPResSo, whereas the reciprocal space part will be computed on the GPU. The results are compared to the existing particle-particle particle-mesh (P3M) algorithm without GPU support. For moderate densities, the GPU-accelerated Ewald summation is comparable in efficiency with the better scaling P3M algorithm up to about 3000 particles, but allows for much higher accuracies without drastic penalties if desired.

CPP 32.8 Tue 14:00 Poster B

**Monte Carlo Studies on dendrimers with special terminal-groups at different solvent conditions** — •Martin Wengenmayr, Jens-Uwe Sommer, and Ron Dockhorn — Leibniz Institute of Polymer Research Dresden, Germany

Monte Carlo Simulations of high generation dendritic polymers at different solvent conditions are performed using the Bond Fluctuation Model on CPU and GPU. Different solvent conditions are applied using explicit solvent. In order to comply with the wide range of dendrimer modifications different terminal groups, for instance flexible linear chains, were attached. Static and dynamic properties like the radius of gyration, the gyration tensor and the conformation of subunits are investigated in detail. We expect that our results help to understand the swelling and collapse of a dendrimer as a carrier molecule for drug delivery processes.

CPP 32.9 Tue 14:00 Poster B

**Comparison of passive and active microrheology for an unentangled polymer melt** — •Anja Kuhnhold and Wolfgang Paul — Martin-Luther-Universität Halle-Wittenberg, Halle, Deutschland

We use molecular dynamics simulations to study the microrheology (MR) of an unentangled polymer melt. Microrheology aims at the estimation of the complex shear modulus of a probe from the motion of suspended micro- or nanoscopic particles in the probe.

This motion can either be purely thermal, similar to the Brownian motion, or forced to a specific form, like an oscillation. The former is called passive MR and the latter active MR.

In passive MR the complex modulus is calculated by using a generalized Stokes-Einstein relation. In active MR a corresponding relation depends on the specific form of the motion.

Our system is a melt of short bead-spring polymer chains including one nanoparticle. For the active MR we use an oscillating harmonical potential, similar to the experimental optical tweezer, to force the particle to oscillate with a certain frequency. Passive and active MR give similar results in the linear response regime independent of temperature, and at high temperatures these are equal to the true (reference) bulk modulus. The lower frequency range is better accessible by passive MR while with active MR one can generally reach higher frequencies.

CPP 32.10 Tue 14:00 Poster B

**Effects of Stiffness on a Generic Polymer Model and where Knots come into Play** — •Martin Marenz and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany

We give an overview of the influence of bending stiffness on the conformational phases of a generic homopolymer model and study especially the occurrence of knots as stable pseudo phases. Thus we present the pseudo-phase diagram for the complete range of semi-flexible polymers, ranging from flexible to stiff ones. Although it is a simplistic model, we have observed a rich variety of conformational phases which are comparable to conformations observed for real polymers and proteins. Just by changing the internal bending stiffness, the polymer model features different pseudo-phases like bended, knot-like, hairpin or toroidal phases. To identify these phases we have calculated, besides standard observables, the complete gyration tensor and the knot type of the polymer via the Alexander polynomial. Due to the relative complex phase space with numerous pseudo-phase transitions and the large parameter space, we used a recently developed parallel variant of the multicanonical algorithm to cope with all problems arising from the transitions and the slow dynamics at very low energies.

CPP 32.11 Tue 14:00 Poster B

**Parallelized Event Chain Algorithm for Dense Hard Sphere and Polymer Systems** — •Tobias Alexander Kampmann, Horst-Holger Boltz, and Jan Kierfeld — TU Dortmund University

We present a parallelized event chain algorithm for hard sphere systems. Analyzing the performance gains for the parallelized event chain in two dimensions we find a criterion for an optimal degree of parallelization. Furthermore we discuss the extension of the algorithm to other systems with hard sphere interactions with a special focus on dense polymeric systems (polymer melts).

CPP 32.12 Tue 14:00 Poster B

**The evaporation of nanodroplet on a heated substrate** — •Jianguo Zhang, Frederic Leory, and Florian Müller-Plathe — TU Darmstadt

Two non-equilibrium methods (called bubble method and splitting method, respectively) developed to study the steady-state evaporation of a droplet surrounded by its vapor, where the evaporation continuously occurs at the vapor-liquid interface while the droplet size remains constant [1]. Then we present our activity dealing with the evaporation of nanometer sized droplets. The evaporation mechanisms of nanodroplets on surface which are chemically both homogenous and heterogeneous are studied by MD simulations under nonequilibrium conditions [2-4].

[1] Zhang, J., Müller-Plathe, F., Yahia-Ouahmed, M., & Leroy F., J. Chem. Phys. (2013), 139, 134701. [2] Zhang, J., Leroy, F. & Müller-Plathe, F., Langmuir (2013), 29, 9770-9782 [3] Zhang, J., Leroy, F. & Müller-Plathe, F., PRL (2014), 113, 046101. [4] Zhang, J., Leroy, F. & Müller-Plathe, F., in preparation.

CPP 32.13 Tue 14:00 Poster B

**Implicit-solvent coarse-grain models of thermosensitive polymers** — •Richard Chudoba[1,2], Jan Heyda[3], and Joachim Dzubiella[1,2] — [1]Dept. of Physics, Humboldt-University Berlin, Germany — [2]Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, Germany — [3]Dept. of Physical Chemistry, Institute of Chemical Technology, Prague, Czech Republic

Functionalized, thermosensitive polymers have become an integral building block for the development of “smart”, environment-sensitive materials with tunable properties. In particular close to their lower critical solution temperature (LCST) copolymers show dramatic changes in their material properties in response to only tiny changes in the solvent environment, e.g. a salt concentration. Solution theory based but still empirical route towards the quantitative prediction of ion-specific effects on polymer folding has been proposed recently.

We employ implicit-solvent coarse-graining strategy to verify this concept on the models of thermosensitive polymers. Our primary targets are poly(ethylene)glycole (PEG) and poly(N-isopropylacrylamide) (PNIPAM), both widely experimentally studied and characterized due to their potential not only in biological applications.

Replica exchange molecular dynamics have been employed to gather equilibrium statistics for polymer in explicit solvent at temperatures around LCST and serve as a reference for the coarse-graining step. The iterative Boltzmann inversion is here the method of choice and the resulting implicit polymer models are then simulated within Monte Carlo and/or Brownian dynamics.

CPP 32.14 Tue 14:00 Poster B

**Two dimensional nanomaterials as sensors and drug delivery agents** — Hakkim Vovusha[1], •Suparna Sanyal[2], and Biplab Sanyal[1] — [1]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden. — [2]Department of Cell and Molecular Biology, Uppsala University, Uppsala, Sweden

Two dimensional nanomaterials have emerged as promising agents for enabling fabrication of data storage devices, sensors for molecular detection, e.g., sensing of gas molecules involved in environmental hazards and drug delivery agents due to their ultrathin size with all surface effects, exotic electronic and mechanical properties. Understanding of electronic structures of these materials is important to design new materials for better sensitivity and selectivity of molecules. In this context, adsorption characteristics of different molecules such as DNA/RNA nucleobases, explosive molecules and polycyclic aromatic hydrocarbons with 2D graphene, graphene oxide, boron nitride and hybrid boron nitride-graphene in both nano flake and infinite 2D sheet geometries have been studied by density functional theory (DFT). Also, time-dependent DFT has been used for calculations of optical properties for identifying features due to adsorption. Our results provide important insights in gas sensing and drug delivery issues.

CPP 32.15 Tue 14:00 Poster B

**About the time dependency of the Van der Waals equation of state** — •Peter Friedel — Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden

The Van der Waals equation is one of the prototypes of the equation of states for realistic systems because of the first time introduction of excluded volume and particle interactions into theoretical considerations. On the other side the simulated annealing (and the similar simulated compressing) approach applies the time dependency to one of the variables of state performing simulations of realistic systems as quasi static state changes. The combination of this time dependency and the VdW-EoS enables a generalization of such considerations up to the simulations of time dependent processes like phase transitions and the obtaining of phase transition kinetics. Simple mathematical deductions starting with the time dependent Van der Waals equation allow the derivation of two so called differential simulated changes of state methods under isobar and isotherm conditions. These new methods enable simulations of crossing phase transition points of hypocritical substances without the danger that the simulations crash because of the achievement of infinite values of the corresponding susceptibility coefficients.

## CPP 33: P5: Microswimmers, Active Liquids

Time: Tuesday 14:00–16:00 Location: Poster C

CPP 33.1 Tue 14:00 Poster C

**Light-driven Microswimmers: Run-and-Tumble depend on the conditions** — •Celia Lozano[1,2], Jannick Fischer[1], Felix Kümmel[1], and Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universität Stuttgart — [2]Max-Planck-Institut für Intelligente Systeme, Stuttgart

Recently, notable improvements regarding the understanding of the dynamics of active particles have been obtained [1]. While their swimming motion under bulk conditions is rather well understood, only little is known about the dynamical properties of active particles under conditions where the Peclet (Pe) number various as a function of the particle position. We present an experimental study, where active motion is achieved by diffusiophoretic forces in a binary solvent and where the Pe number is controlled by the light intensity [2]. In the presence of one-dimensional periodic intensity patterns, we observe the accumulation/depletion of active particles in regions with low/high illumination, i.e. with small/large Pe numbers. We study the steady state particle density variations as a function of the ratio of the persistence length of active particles and the strip width of the intensity pattern and compare our results to numerical simulations. We expect, that our findings contribute to the understanding of pattern formation of chemotactic organisms in chemical gradients.

[1] B. ten Hagen, F. Kümmel, R. Wittkowski, D. Takagi, H. Löwen, and C. Bechinger Nature Comm. 5, 4829 (2014) [2] I. Buttinoni, G. Volpe, F. Kümmel, G. Volpe, and C. Bechinger J. Phys.: Cond. Mat. 24, 284129 (2012)

CPP 33.2 Tue 14:00 Poster C

**Self-propulsion of Janus particles near a polymer functionalized surface** — •Mojdeh Heidari and Regine von Klitzing — Stranski Laboratorium für Physikalische und Theoritische Chemie, Inst. für Chemie TU Berlin, Straße des 17. Juni, 10623 Berlin, Germany

Active colloidal suspensions are consisting of particles with dimensions ranging from hundreds of nanometer to tens of micrometer. These particles are able to move autonomously under out-of-equilibrium conditions by converting the energy of their environment into directed motion. So far, the motion of microswimmers has been investigated close to a glass slide, whereas the interactions between particles and the substrate are often neglected. However, these interactions are expected to play a significant role in the motion of microswimmers.

In this study we explore the motion of Janus-type microswimmers close to a glass slide which is functionalized with thermoresponsive PNIPAM brushes. Janus particles are polystyrene microbeads half coated with Au and undergo self-propulsion by taking advantage of thermophoretic effect under laser illumination. The remarkable advantage of such Janus particles is that their self-propelled motion can be switched on and off on demand by adjusting laser intensity. Structural properties of polymer brush layer on the substrate such as roughness, thickness and grafting density has been varied and the respective influence of such variations on the motion of microswimmers has been addressed.

CPP 33.3 Tue 14:00 Poster C

**Active microrheology in colloidal soft-matter** — •Robert Wulfert[1], Udo Seifert[1], and Thomas Speck[2] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany

Tracking the microscopic motion of a driven colloidal probe through a complex host medium delivers valuable insight regarding the system's dissipative behaviour in the non-linear response regime. The active forcing disturbs the equilibrium microstructure around the probe causing an excess of particles in front and a depopulated wake trailing it. This anisotropy in the pair-distribution corresponds to a frictional drag on the probe due to colloidal interactions, which can be interpreted in terms of an effective viscosity on the micron-scale. We calculate the pair-distribution function from the pair-Smoluchowski equation for hard-sphere colloids with additional long-range interactions. Furthermore, we discuss how the resulting velocity-force relations generalize in the case of dense and hence strongly interacting host suspensions and compare our results to Brownian dynamics simulations.

CPP 33.4 Tue 14:00 Poster C

**From Single Artificial Self-Propelled Particles to Collective Motions** — •Leonard Li[1], Ralf Seemann[1,2], and Jean-Baptiste Fleury[1] — [1]Saarland University, Experimental Physics, Saarbruecken, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany

Collective motions as manifestation of a coordinated behavior are commenly observed in living-organisms: from bacteria to birds, sheaps and fishs. Recently, identical type of behavior could be also observed with non-living system, i.e swarmming of self-propelled droplets dancing into a microfluidic chip. Based on this type of system, we study the conditions leading to the emergence of collective motion from the hydrodynamic interaction between individual self-propelled objects.

CPP 33.5 Tue 14:00 Poster C

**Quantifying random walk properties of Caenorhabditis elegans with the WormTracker** — •Carsten Schade and Matthias Weiss — Universität Bayreuth

The locomotion pattern of C. elegans (a small transparent roundworm)is complex and depends on the visco-elastic properties of the environment. Here, we have used a custom-made worm imaging platform to monitor the random walks of individual worms in varying environments. As a result, we have observed that the probability distribution of spatial increments depends on the visco-elastic properties of the worm's environment. Moreover, these probability distributions Show signatures of Levy-stable distributions, hence suggesting near-optimal search strategies to explore the environment.

CPP 33.6 Tue 14:00 Poster C

**Swimming Dynamics of *C. reinhardtii* in Confined Geome-**

**tries** — •Tanya Ostapenko, Christian Kreis, and Oliver Bäumchen — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Fassberg 17, 37077 Göttingen, Germany

*Chlamydomonas reinhardtii* is a unicellular, biflagellated alga that has long been appreciated as a model organism in biology. Recently, their possibilities as a source of therapeutic proteins and renewable biofuels have attracted much interest. Previous research in the physics community to date has mainly focused on the propulsion mechanism of this microswimmer in bulk, as well as quasi-two-dimensional systems. Recently, the influence of interfaces on the dynamics has been recognized as an important factor. Additional studies showed that active swimmers affect the rheological (*e.g.* the effective viscosity) and transport properties of dense suspensions.

We report on the behavior of *C. reinhardtii* in two different, confined environments. First, we consider cells injected into a quasi-two-dimensional microfluidic chip, where we find that the geometric shape and dimensions in which the cells swim can affect their trajectories and wall interactions. Secondly, we investigate *C. reinhardtii* in an evaporating droplet, where the volume in which the cells may swim is time-dependent. We discuss possible explanations for any resulting pattern formations, as well as how the confined environment impacts the swimming dynamics.

CPP 33.7 Tue 14:00 Poster C

**Bacterial swimming in narrow spaces** — •Marius Hintsche, Michael Raatz, Marco Bahrs, Matthias Theves, and Carsten Beta — Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany

The natural habitat of many bacterial swimmers is dominated by interfaces and narrow interstitial spacings. Thus, they will often interact with the fluid boundaries in their vicinity. To quantify these interactions, we investigated the swimming behavior of the soil bacterium Psudomonas putida in a variety of confined environments. We fabricated structured microchannels with different configurations of cylindrical obstacles as well as unstructured narrow chambers. In these environments we recorded swimming trajectories and measured key motility parameters for different obstacle densities and arrangements. Although the run-and-turn swimming pattern does not change, the shape of trajectories varies in different obstacle configurations. Motility parameters like speed, run times and turning angles depend strongly on the obstacle density. This is likely to be a combination of hydrodynamic wall effects and collisions with the obstacles.

CPP 33.8 Tue 14:00 Poster C

**Modeling active systems on different length scales: a comparison of pattern phenomenology** — •Jonas Denk, Lorenz Huber, Emanuel Reithmann, and Erwin Frey — Ludwig-Maximilians-Universität, München, Deutschland

Modeling complex biological systems always includes a level of coarse-graining in order to reduce the intricate functions of each microscopic constituent and their interplay to a comprehensive description. For active systems of self-propelled particles realizations of this coarsening procedure range from agent-based simulations on a single particle level to mean field descriptions on a hydrodynamic length scale. Because these two approaches are conceptually different it is important to ask whether they yield similar results especially with respect to the formation of macroscopic patterns. Motivated by recent *in vitro* experiments of membrane-bound FtsZ, a bacterial cell-division protein, we compare microscopic particle-based simulations to a coarse-grained kinetic Boltzmann approach for systems of chirally driven polymers. We discuss conceptual differences and identify observables, that are suited for each level of description. We find that both approaches exhibit the same phenomenology in terms of vortex structure and flocking states. Furthermore, we argue discrepancies between them and discuss possible applications in the field of self-propelled particle systems.

## CPP 34: P6: Biomaterials and Biopolymers

Time: Tuesday 14:00–16:00 Location: Poster C

CPP 34.1 Tue 14:00 Poster C

**Nanoscale viscoelastic properties of hydrated collagen-based films probed with static and dynamic AFM** — •Manuel Uhlig, Eike-Christian Spitzner, and Robert Magerle — Chemische Physik, Fakultät für Naturwissenschaften, TU Chemnitz, 09107 Chemnitz, Germany

The amount and distribution of water in collagen-based films determines their mechanical properties and shape. We investigate the effect of hydration on reconstituted collagen fibrils and gelatin films (i.e., denaturated collagen) by controlling the relative humidity of the surrounding air. Measurements are performed with atomic force microscopy (AFM) including static and dynamic force spectroscopy as well as stress relaxation experiments. By combining these methods, the mechanical response is characterized over a wide range of time scales. We obtain maps of the specimen's viscoelastic properties in the near-surface region. For each material, one single AFM probe (Si, with a force constant of 15 N/m) is used during the entire experiment, thus allowing comparison of different tip-sample interaction mechanisms. Gelatin films show a distinct, humidity induced transition from a stiff to a compliant, viscoelastic state. In contrast, collagen fibrils soften more gradually with increasing relative humidity.

CPP 34.2 Tue 14:00 Poster C

**A pressure-dependent FTIR-spectroscopy study on spider silk's non-equilibrium nanostructure** — •Arthur Markus Anton[1], Christof Gutsche[2], Wilhelm Kossack[1], and Friedrich Kremer[1] — [1]Institut für Experimentelle Physik I, Universität Leipzig, Germany — [2]Poliklinik für Zahnerhaltung und Parodontologie, Universität Leipzig, Germany

To investigate the molecular structure and the interaction between internal and external constraints in spider silk a pressure dependent analysis by means of a diamond anvil cell (DAC) has been carried out. On the one hand, the spectral shift of a structure-specific IR-absorption band provides evidence of the inherent non-equilibrium nanostructure in spider silk, as composed of alanine-rich nanocrystals embedded in a glycine-rich and *prestressed* amorphous matrix [A. M. Anton et al., *Macromol.* **46** (2013)]. On the other hand, combining polarization-dependent IR-transmission and optical microscopy measurements allows for separating between order and disorder at macroscopic and microscopic scales for a variety of (bio)macromolecular fibers. Thus, on the example of spider silk the molecular order parameter of the alanine building blocks is determined and found to decrease reversibly by 0.01 $\mathrm{GPa}^{-1}$ when varying the external hydrostatic pressure between 0 and 3 GPa [A. M. Anton et al., *manuscript submitted*].

CPP 34.3 Tue 14:00 Poster C

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

During times of environmental stress (e.g., UV or heat exposure), levels of reactive oxygen species (ROS) can increase. This may result in significant damage to cell structures. Here we focus on the effect of hydroxyl radicals (produced by Fenton reaction) on model membranes. Combining isotherms, X-ray diffraction, X-ray reflection and IRRAS, we find a partial cleavage of the head group leading to a reduced head group size with negative charge for DPPC monolayers at the air/water interface. Free iron ions are produced by the Fenton reaction, they bind to the head group. Fluorescence microscopy showed immediate nucleation of new domains in the condensed phase, followed by solidifcation. Similar effects are observed with differential scanning calorimetry and confocal microscopy for DMPC liposomes. The use of EDTA in high excess to catch all free iron ions prevents the solidification of the monolayers and liposomes. The chemical changes of the lipids due to radical attack have no direct effect on the phase transition and solidification. Solidification and destruction of the model membranes after the Fenton reaction are attributed to the iron ions, which bind very strongly to the lipids after the radical attack.

CPP 34.4 Tue 14:00 Poster C

**Synchrotron Radiation- based FIR/THz spectroscopy for studying Membrane-targeting interactions of antimicrobial peptides** — •Andrea Hornemann[1], Arne Hoehl[1], Michael Andersch[1,2], Peggy Emmer[1], Michael Vollmer[2], Gerhard Ulm[1], and Burkhard Beckhoff[1] — [1]Physikalisch-Technische Bundesanstalt, Berlin, Germany — [2]University of Applied Sciences in Brandenburg, Brandenburg, Germany

The development of new infrared radiation sources has initiated opportunities for exploring the molecular structure of many (bio-) materials in the far-infrared/terahertz spectral region. The identification of thin organic films derived from peptide layers at polymer/organic interfaces was performed by Synchrotron Radiation (SR-) based FTIR spectroscopy at PTB's Metrology Light Source. For bioanalytical applications, the FIR/THz spectroscopic technique offers a unique tool for a distinct identification of biochemical components by their vibrational spectra. Peptide films were studied in the spectral region from 400 $\text{cm}^{-1}$ to 5 $\text{cm}^{-1}$. This spectral region complements the mid-infrared spectral range where molecules such as proteins deliver characteristic modes, and entails additional molecular information on torsion and bending modes of the carbon backbone and H-bonds of biomolecules. We discuss the signatures of different membrane-targeting antimicrobial peptides that display defined secondary-structure motifs. Our approach entails T-dependent studies between between 298 K and 10 K.

CPP 34.5 Tue 14:00 Poster C

**An x-ray diffraction study of vulcanized fiber and paper exposed to hydrostatic pressure** — •Karin Esch[1], Dominik Dumke[2], Michael Paulus[1], Christian Sternemann[1], Julia Nase[1], Julian Schulze[1], Johannes Möller[1], Kolja Mende[1], Irena Kiesel[1], Thomas Büning[1], Simon Wulle[1], Sergius Janik[1], Holger Göring[1], Dorothee Wieczorek[2], and Metin Tolan[1] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, D-44221 Dortmund, Germany — [2]Fakultät Maschinenbau, Technische Universität Dortmund, D-44221 Dortmund, Germany

Vulcanized fiber, consisting of cellulose, is a material of various applications. It is used as an insulator in electrical industry, and can be found in washers/gaskets and welding shields. As vulcanized fiber and paper are made from renewable resources, these materials gained increasing interest in recent years. A way to produce vulcanized fiber is parchmentising. Raw paper is soaked with a $ZnCl_2$ solution, pressed, rested for a certain time, and washed out in steps of descending concentrations. Paper consists mostly of cellulose $I_\alpha$ and $I_\beta$. During the process of parchmentising cellulose I transforms to cellulose II and changes the material's structure on a molecular level. Consequently, macroscopic properties change, e.g. the material becomes harder and stiffer. The underlying structural changes can be analysed by x-ray diffraction. We studied changes in the diffraction pattern of paper and vulcanized fiber at high hydrostatic pressure up to 4 kbar. An anisotropic reversable compression was found. The experiments were performed at beamline BL9 of the synchrotron lightsource DELTA, Dortmund.

CPP 34.6 Tue 14:00 Poster C

**AFM studies of adsorbed xylan on cellulosic materials** — •Caterina Czibula[1,2], Christian Ganser[1,2], Albrecht Miletzky[2,4], Stefan Spirk[3], Robert Schennach[2,5], and Christian Teichert[1,2] — [1]Institute of Physics, Montanuniversitaet Leoben, Austria — [2]Christian Doppler Laboratory for Surface Chemical and Physical Fundamentals of Paper Strength, Graz University of Technology, Austria — [3]Institute for Chemistry and Technology of Materials, Graz University of Technology, Austria — [4]Institute for Paper-, Pulp- and Fibre Technology, Graz University of Technology, Austria — [5]Institute of Solid State Physics, Graz University of Technology, Austria

Xylan is the predominant hemicellulose in plants and wood. It is a byproduct in papermaking and the production of regenerated cellulose fibers. To find an additional use of xylan, its ability to positively influence mechanical properties of paper is investigated at the example of a variety of cellulosic substrates. The adsorption of xylan to amorphous cellulose thin films, viscose fibers, and paper fibers is studied. Atomic force microscopy (AFM) is employed to characterize the topography of the samples and to analyze their surfaces. The size of the randomly distributed xylan aggregates varies between 20 nm - 30 nm. The shape, either globular or elongated, is dependent on the electrolyte concentration.

CPP 34.7 Tue 14:00 Poster C

**The adsorption of a cellulose binding module on cellulose surfaces** — •Sergio Mauri[1], Jim Pfaendtner[2], Mischa Bonn[1], and Tobias Weidner[1] — [1]Max Planck institute for polymer research, Mainz, Germany — [2]Dept. of chemical engineering, University of Washington, Seattle, US

The conversion of biomass, like other biological processes, is rate-controlled by interfacial phenomena. In the case of enzymatic biomass conversion, cellulose enzymes present specific carbohydrates binding modules (CBM) to provide an increase in concentration of enzyme sites near the cellulose interface. Here we propose to study the interaction of a CBM with cellulose surfaces by a combination of methods, to quantify the adsorption of CBM on cellulose surfaces and to elucidate the CBM/cellulose interfacial structure. We follow the concentration dependent adsorption kinetics of CBM on cellulose surfaces by means of QCM-D and we determine the Langmuir adsorption isotherm. On the same substrate we perform XPS to compare wet and dry adsorbed mass. We finally determine the orientation of the adsorbed protein on such cellulose surfaces by using sum frequency spectroscopy (SFG). SFG is a nonlinear optical technique which provides surface-specific vibrational spectra of sub-monolayers of interfacial molecules. SFG, in conjunction with simulation results, is well-suited for determining the orientation of CBM on cellulose surfaces.

CPP 34.8 Tue 14:00 Poster C

**Determination of Amylolytic Activityof Malts by Rheological Measurements** — •Janyl Iskakova, Jamila Smanalieva, and Asylbek Kulmyrzaev — Kyrgyz-Turkish Manas University, Bishkek, Kyrgyzstan

Malting is the most important stage in the processing of the Kyrgyz traditional beverage Bozo. In current study, the amylase activities of maize, millet, wheat, and barley malts were investigated by rheological methods using cooked millet porridge as a substrate for enzymes.

The aim of this work has been to demonstrate the applicability of rheological measurements as alternative, rapid, safe for health and simple method for measuring amylolytic activity of grain malts. The standard colorimetric method for the determination of amylase activity was compared with rheological method. Millet porridge exhibited pseudoplastic behavior and the Ostwald-De-Waele was used as suitable fitting model. The highest amylolytic activity was found in barley malt and the lowest in maize malt. The rheological method is demonstrated to be advantageous, particularly with regard to speed, simplicity, no requirement for chemicals and possibility of the online monitoring of the structural changes.

CPP 34.9 Tue 14:00 Poster C

**A polyethylene glycol / $\gamma$-globulin mixture as a versatile depletion interaction system for the study of crowding effects** — •Stefano Da Vela[1], Fajun Zhang[1], Christian Exner[1], Saliba Barsaume[1], Michael Sztucki[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]ESRF, Grenoble, France

Bovine $\gamma$-globulin is a polyvalent antibody preparation consisting mainly of Immunoglobulin G (IgG), an anisotropic, Y-shaped protein. Solutions of $\gamma$-globulin, with polyethylene glycol (PEG) of variable molecular weights added as depletion agent, can be used as a model to study the effect of attractive particle-particle interactions with tunable range and strength. The phase behaviour is comparable to that of monoclonal antibody systems, with the appearance of a gas-liquid coexistence region accessible above the freezing temperature of water, within a range of PEG concentrations. However, the availability of large amounts of protein in the case of $\gamma$-globulin allows for an extensive exploration of its phase diagram: regions at high protein volume fraction and the possibility to realize arrested phase transitions are of particular interest. Moreover, by choosing appropriate PEG molecular weights and concentrations, the phase behaviour can be described in conditions beyond those of applicability of the Asakura-Oosawa model of depletion interactions. Typical phase diagrams as a function of PEG concentration and temperature are presented, while dynamic light scattering and small-angle x-ray scattering are employed to characterize the interaction.

CPP 34.10 Tue 14:00 Poster C

**Diffusion in protein solutions upon approaching a liquid-liquid phase transition and its critical point** — •Michal Braun, Marcell Wolf, Fajun Zhang, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen

We study aqueous solutions of globular proteins and multivalent salts ([1], [2], [3]). In the bovine serum albumin (BSA) system with $YCl_3$ liquid-liquid phase separation (LLPS) occurs in a certain region of the phase diagram. We performed temperature dependent dynamic light scattering measurements to monitor the diffusion behavior upon approaching the liquid-liquid phase transition. We found two contributions to the collective diffusion. The faster diffusion is ascribed to small clusters whereas the slower contribution is due to collective diffusion of larger clusters. Both the slow and fast collective diffusion coefficients first increase as expected according to the Stokes-Einstein equation. Upon approaching the phase transition they decrease linearly due to the formation of clusters. A new theoretical model is needed to explain these experimental observations. The Rayleigh ratio as well as the diffusion coefficients may be used to estimate the spinodal and binodal temperatures of the system. The classification of the critical behavior turns out to not be as straightforward as in the case of other binary systems. This is due to the formation of clusters before the onset of phase transition. [1] Zhang et al., *PRL*, **101**, 148101, 2008, [2] Zhang et al., *Soft Matter*, **8**, 1313, 2012, [3] Roosen-Runge et al., *PNAS*, **108**, 11815, 2011

## CPP 35: P7: Hydrogels and Elastomers

Time: Tuesday 14:00–16:00 Location: Poster C

CPP 35.1 Tue 14:00 Poster C

**Demixing transition and molecular interactions in poly(N-isopropyl acrylamide) compared to its monomer** — •Moritz Futscher[1], Martine Philipp[1], Peter Müller-Buschbaum[1], and Alfons Schulte[2] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]University of Central Florida, Department of Physics, The College of Optics & Photonics, Orlando, Florida 32817-2385, US

Temperature-sensitive hydrogels such as poly(N-isopropyl acrylamide) (PNIPAM) exhibit a coil to globule transition of the polymer chains with a lower critical solution temperature (LCST) near 32 °C. The cooperative dehydration of bound water molecules upon heating plays a significant role. The hydrogen bonding with the amide groups in the side chains has to be contrasted with the hydration interaction of the hydrophobic main chain hydrocarbons. Employing FTIR spectroscopy we probe molecular changes in the various chemical groups. PNIPAM and its monomer NIPAM are investigated at a concentration of 20 wt% in aqueous solution. We observe a nearly discontinuous shift of the peak frequencies and the intensities of vibrational bands (amide I, amide II, CH) in PNIPAM, while in NIPAM there is a continuous linear shift with temperature. The results are discussed with respect to hydration changes in the amide group and cooperative interactions with bound water along the backbone chain.

CPP 35.2 Tue 14:00 Poster C

**The Formation and Swelling of Superabsorbent Networks: A Monte Carlo Study** — •Michael Lang, Andreas John, and Jens-Uwe Sommer — Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Straße 6, 01069 Dresden, Germany

The free-radical polymerization was studied in aqueous acrylic acid solution in the presence of cross-linkers using the Bond Fluctuation Model (BFM). Network formation was analyzed for varying cross-linker reaction rates, cross-linker composition and number fraction, cross-linker functionality and time dependent initiator release. For all simulations we observe an auto-acceleration of reaction kinetics similar to the gel effect but independent of the degree of cross-linking. The weight distributions of chains that result from reactions of one radical and the number distribution of cross-linkable sites on these chains can be approximated by Poisson distributions. The weight fractions of the active material and gel, the average strand length within the active material, and the gel point are determined. The swelling behavior of neutralized networks seems to confirm the Flory-Rehner prediction for the equilibrium degree of swelling as function of the average strand length. However, a more detailed investigation reveals that this results from the fortuitous cancellation of corrections due to inactive material and entanglements for networks with a structure similar to our study. Thus, only the networks with a rather large active strand length agree with the Flory-Rehner model, while the networks with a short elastic strand length show an additional non-affine contribution to the equilibrium degree of swelling.

CPP 35.3 Tue 14:00 Poster C

**Single and double networks from amphiphilic star block copolymers** — •Xiaohan Zhang[1], Konstantinos Kyriakos[1], Elina N. Kitiri[2], Maria Rikkou-Kalourkoti[2], Costas Patrickios[2], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Soft Matter Physics Group, Garching — [2]University 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. To improve the mechanical strength, especially regarding compression, a second hydrophilic polymer network is introduced into these amphiphilic networks.

We investigate amphiphilic conetworks from various acrylic blocks which differ in composition, water solubility and mechanical properties. We have studied the structures of the single and the conetworks using small-angle X-ray scattering which reveals information about the microphase-separated morphology. We find that their degree of swelling in water as well as the underlying mesoscopic structures depend strongly on these characteristics.

CPP 35.4 Tue 14:00 Poster C

**Light induced phase transitions in gold-microgel hybrids** — •Maren Lehmann, Sarah Turner, Lucas Kuhrts, and Regine von Klitzing — Stranki-Laboratory, Dept. of Chemistry, TU Berlin, Germany

Poly(N-isopropylacrylamide) (PNIPAM) microgels are one of the most studied soft materials. They respond to various external stimuli, which makes them attractive for biological applications, such as drug delivery and biosensing, as well as for catalysis or nanoreactors [1] [2]. Depending on their composition PNIPAM microgels respond to pH, ionic strength or solvent. By introducing metal nanoparticles they are able to react to a magnetic field or light. We incorporated gold nanoparticle into the microgel network in order to introduce a responsiveness to light of the plasmon resonance wavelength of the gold nanoparticles. The temperature dependent size of the microgel and the hybrids was measured by dynamic light scattering (DLS). The swelling and shrinking properties were investigated by DLS and temperature-controlled UV-Vis adsorption spectroscopy. The uptake of gold nanoparticles per microgel particle and their distribution within the microgel particles were studied with the transmission electron microscope.

[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)

CPP 35.5 Tue 14:00 Poster C

**Finite element analysis of filled elastomer networks responding to static external stress** — •Sergej Berdnikow and Reinhard Hentschke — Bergische Universität, 42279 Wuppertal, Germany

Technical elastomers acquire most of their mechanical strength through fillers forming spanning branched networks throughout the elastomer matrix. Depending on filler concentration and processing conditions the filler network may consist of fractal flocs, giving rise to the unique and often desirable mechanical properties of rubber materials. Here we present a finite-element based model of filler networks embedded in an elastic matrix subjected to a static external stress. It is calculated how the network responds to the rupture of highly loaded network junctions caused by the external forces. We compare quasi-fractal filler networks, i.e. filler networks possessing fractal structure below a certain length scale, which are often found in for instance tire tread materials, to random filler networks at otherwise identical conditions. We observe that the so called "occluded rubber" effect, which is present for the quasi-fractal networks, is destroyed upon random reordering of the filler. In addition, significant load redistribution during filler network damage can be seen when the filler structure is quasi-fractal. For random fillers this load redistribution is almost completely absent.

# CPP 36: Organic Electronics and Photovoltaics: OPV II (joint session CPP, HL, TT)

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

CPP 36.1 Wed 9:30 C 130

**Impact of Mesoscale Order on Energetics in Organic Semiconductors** — •Carl Poelking[1], Max Tietze[2], Chris Elschner[2], Selina Olthof[3], Dirk Hertel[3], Björn Baumeier[1], Frank Würthner[4], Klaus Meerholz[3], Karl Leo[2], and Denis Andrienko[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Institut für Angewandte Photophysik, Dresden, Germany — [3]Physikalische Chemie, Universität zu Köln, Germany — [4]Institut für Organische Chemie, Universität Würzburg, Germany

The interaction of charged excitations with the molecular surrounding in organic semiconductors is strictly long-ranged, due to their quadrupolar building blocks and preferential or absolute structural order. We show how atomistic simulations access the resulting energetics of charges and charge pairs and derived quantities, notably the charge-density-dependent open-circuit voltage across organic heterojunctions, with excellent accuracy. We compute level diagrams for a variety of donor-fullerene interfaces, with direct experimental validation. The underlying simulation approach takes into account long-range electrostatic effects that persist up to the mesoscale. The resulting mesoscale fields not only produce flat level profiles, but provide orientation-dependent push-out forces across a donor-acceptor interphase that can drive the charge-separation process. Correct polarity of these push-out forces is a requirement for functional solar cells, with operation closely above an isopolar point as the optimum tradeoff between magnitude of these push-out forces and the photovoltaic gap.

CPP 36.2 Wed 9:45 C 130

**Signature of the Dirac cone in the excitation gaps of linear oligoacenes** — •Richard Korytár — Institut für Nanotechnologie, Karlsruher Institut für Technologie, Herrmann-von-Helmholtzplatz 1, 76344 Eggenstein-Leopoldshafen

Linear oligoacenes (linearly fused benzene rings) are one of the prototypical examples of quantum wires and the simplest realization of the so called nano-graphene. We show that contrary to a widely held belief, the excitation gaps of oligoacenes can display oscillations of period 11 (rings) as a function of the molecule's length. By inspection of the polyacene electronic band-structure, we show that the incommensurate oscillations are caused by the presence of an accidental degeneracy at the Fermi level, reminiscent to the Dirac cone of graphene. Our predictions are supported by calculations based on density functional theory. We clarify the role of interactions by studying a parameterized Hubbard model with density matrix renormalization group. Our findings may have implications for organic electronics and research of materials for energy conversion.

CPP 36.3 Wed 10:00 C 130

**Probing Interfacial Properties in Polymer:Fullerene Bulk Heterojunctions** — •Christian Kästner[1], Daniel A. M. Egbe[2], and Harald Hoppe[1] — [1]Institute of Physics, Technische Universität Ilmenau, Ilmenau, Germany — [2]Linz Institute for Organic Solar Cells, Johannes Kepler University, Linz, Austria

We investigated the properties of donor-acceptor interfaces occurring in fine-tuned ternary bulk heterojunctions and were able to quantitatively correlate spectroscopic information with domain phase order. Relaxation energies for AnE-PV donor polymers as well as of PCBM were found to range within 100-200 meV.

CPP 36.4 Wed 10:15 C 130

**The Effect of Solvent Additive on Generation, Recombination and Extraction in PTB7:PCBM Solar Cells: A conclusive Experimental and Numerical Simulation Study** — •Juliane Kniepert[1], Ilja Lange[1], Thomas Brenner[1], Jan Anton Koster[2], and Dieter Neher[1] — [1]Universität Potsdam, Germany — [2]University of Groningen, The Netherlands

Time delayed collection field (TDCF), bias amplified charge extraction (BACE) and space charge limited current (SCLC) measurements are combined with complete numerical device simulations to unveil the effect of the solvent additive 1,8-diiodooctane (DIO) on the performance of PTB7:PCBM bulk heterojunction solar cells. DIO is shown to increase the charge generation rate, reduce geminate and bimolecular recombination and increase the electron mobility. In total, the reduction of loss currents by processing with the additive raises the power conversion efficiency of the PTB7:PCBM blend by a factor of almost three. Our device simulations show unambiguously that the effect of the additive on the shape of the current-voltage curve cannot be ascribed to the variation of only the mobility, the recombination or the field-dependence of generation. It is only when the changes of all three parameters are taken into account that the simulation matches the experimental J-V-characteristics under all illumination conditions and for a wide range of voltages.

CPP 36.5 Wed 10:30 C 130

**Quantification of loss channels in bulk heterojunction organic solar cells based on DPP-type donor-acceptor copolymers blended with PC71BM** — •Julian Robert Ochsmann[1], Deepak Chandran[2,3], Kwang-Sup Lee[3], and Frédéric Laquai[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Dublin City University, Dublin, Ireland — [3]Hannam University, Daejeon, South Korea

A promising approach to improve the performance of bulk-heterojunction (BHJ) organic solar cells (OSC) is to use low-bandgap polymers as electron donor materials as they enhance the photon absorption of the photoactive layer in the near infrared wavelength range and thereby increase the photocurrent. In addition, low-bandgap polymers are suitable for use in tandem solar cells, since their absorption spectrum is complementary to that of mid-bandgap polymers such as P3HT or PCDTBT, which allows for photocurrent matching of front and back cells. A promising class of low-bandgap polymers for single- and multijunction solar cells are donor-acceptor type copolymers based on diketopyrrolopyrrole (DPP) units. In this study we investigate the photovoltaic performance and the photophysics of two DPP-based copolymers, namely PTDPP-TT and PFDPP-TT, blended with PC71BM and applied in single junction BHJ solar cells. The photophysics of the OSC devices were investigated with broadband transient absorption pump-probe spectroscopy (TA) and analyzed with a previously reported model of charge recombination that allows to quantify the loss channels in devices.

CPP 36.6 Wed 10:45 C 130

**Efficiency-Limiting Processes in Low-Bandgap Polymer:Perylene Diimide Photovoltaic Blends** — •Dominik Gehrig[1], Steffen Roland[2], Ian Howard[1], Dieter Neher[2], and Frédéric Laquai[1] — [1]Max-Planck-Institut für Polymerforschung, Mainz — [2]Institut für Physik und Astronomie, Physik weicher Materie, Universität Potsdam

In this work, we present a photophysical study on blends of a low-bandgap polymer, namely PBDTTT-C, as donor in combination with a PDI-based electron acceptor.[1] Exciton and charge carrier dynamics as well as loss mechanisms are investigated by sub-picosecond to microsecond pump-probe transient absorption (TA) and time-resolved photoluminescence (TRPL) spectroscopy in combination with multivariate curve resolution (MCR) data analysis. A largely diffusion-limited exciton dissociation at the donor acceptor interface and consequently a slow charge generation is observed. Time-delayed collection field (TDCF) experiments reveal a strongly field-dependent charge generation process in turn leading to low fill factors in devices. However, once free charges are generated they recombine non-geminately on a ns-us timescale indicating that they can be potentially extracted as photocurrent. By comparison of the PBDTTT-C:PDI charge generation efficiency with that of a PBDTTT-C:fullerene blend, we identify inefficient charge generation and fast non-geminate recombination competing with charge extraction to be the main bottlenecks of photocurrent generation in the investigated polymer:PDI blends.

[1] Gehrig et al., J. Phys. Chem. C 2014, 118, 20077

CPP 36.7 Wed 11:00 C 130

**Effect of solvent vapor annealing on perylene-based solar cells** — •Stefan Grob[1], Mark Gruber[1], Andrew Bartynski[2], Theresa Linderl[1], Mark Thompson[2], and Wolfgang Brütting[1] — [1]University of Augsburg, Augsburg, Germany — [2]University of Southern California, Los Angeles, USA

Diindenoperylene (DIP) and Tetraphenyldibenzoperiflanthene (DBP) are two common materials used in organic solar cell devices. While DIP is growing crystalline, showing good charge and exciton transport but only weak absorption, DBP exhibits an amorphous character, leading to lower carrier mobility and a short exciton diffusion length, however, DBP reveals a distinctly higher absorption. For both materials we investigate the influence of solvent vapor annealing (SVA) on solar cell performance. In general, SVA leads to a reorganization of the treated materials due to a partial re-solubilization of the layers, allowing the molecules to rearrange into structures characterized by a higher degree of order [1]. Though, for DBP, extended annealing times lead to a strong aggregation of the molecules, resulting in inhomogeneous layers unfavorable for solar cells. For DIP cells however, SVA leads to an increase in fill factor (FF) and also a slight increase in short-circuit current density (Jsc) due to interface roughening. Nevertheless, the best results are obtained by combining annealed DIP layers with strongly absorbing DBP and C70 on top. Thereby, we obtain the same increase in FF but a higher gain in Jsc, elevating the power conversion efficiency by almost 20 % up to more than 4 %.

[1] G. De Luca et al., J. Mater. Chem., 2010, 20, 2493-2498

**15 min. break**

CPP 36.8 Wed 11:30 C 130

**Morphology Tuning by Side-chain Variation in Bulk-Hetero-Junction Solar Cells Based on Merocyanines** — •Dirk Hertel, Julian Nowak, Stephanie Rüth, Ruth Bruker, Jürgen Schelter, and Klaus Meerholz — Universität zu Köln, Department Chemie, Luxemburgerstrasse 116, 50939 Köln

Organic photovoltaics (OPV) offers the potential of mass-produced renewable energy. Within the last decade the efficiency of organic solar cells has increased from 3 % to 10 %, mainly based on better understanding and control of morphology. We investigate merocyanines (MC), a class of low-molecular-weight colorants, as donor material in organic solar cells. These molecules are processable via both deposition techniques showing remarkable power conversion efficiencies (PCE) beyond 4% for SOL- and 6% for VAC-processed devices. Despite these impressive numbers the understanding of the influence of morphology on charge generation, transport and recombination in MCs is in its infancy. To aim towards even higher PCEs we have systematically varied the side-chain of a prototypical donor-acceptor MC with a high ground state dipole moment. By applying atomic-force mircroscopy, transmission electron microscopy and x-ray diffraction we are able to elucidate the thin film structure and show how side-chain variation reduces domain size and improves device data. We are able to correlate crystal size to optical, morphological and device data. There is an optimum side chain length and contrary to previous observations the MC:PCBM blend layers processed from solution perform better in OPVs than layers processed by thermal deposition under vacuum.

CPP 36.9 Wed 11:45 C 130

**Exploring the performance enhancement potential of the tapering technology for block-copolymer solar cells using a novel particle-based multiscale solar-cell algorithm** — Anton Pershin, Sergii Donets, and •Stephan Baeurle — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, 93040 Regensburg, Deutschland

Tapered block copolymers offer an exciting opportunity to tailor the interfacial region between different components by conserving their phase-separated mesoscale structure, which enable the generation of polymer systems with the desired spatio-dynamic properties. In this presentation, we explore their usefulness for optimizing the photovoltaic performance of polymer bulk heterojunctions. To this end, we apply a recently developed particle-based multiscale solar-cell algorithm [1,2] and investigate the effect of random tapering at the chemical junctions between the electron-donor- (D) and electron-acceptor- (A) blocks on the photovoltaic properties of various lamellar-like polyfluorene-based block-copolymer systems. Our simulation results [2] reveal that introducing a tapered middle block with optimal length leads to a significant increase of the exciton dissociation efficiency, but deteriorates the charge transport efficiency only moderately. This results in a gain of the internal quantum efficiency from 25 up to 39 % by increasing the thickness of the active layer of the solar cell from 10 up to 50 nm in direction to the DA interface. Literature: [1] A. Pershin, S. Donets, S.A. Baeurle, Polymer 55, 3736 (2014); [2] A. Pershin, S. Donets, S.A. Baeurle, Polymer 55, 1507 (2014).

CPP 36.10 Wed 12:00 C 130

**Effect of alcohol treatment on the morphology and performance of PTB7:PC71BM bulk heterojunction solar cells** — Shuai Guo[1], Biye Cao[1], Weijia Wang[1], Jean-Francois Moulin[2], and •Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]Helmholtz-Zentrum Geesthacht am MLZ, Lichtenbergstr. 1, 85747 Garching

The environmentally friendly alcohol treatment of bulk heterojunction (BHJ) polymer solar cells using the low bandgap copolymer based on thieno[3,4-b]thiophene-alt-benzodithiophene units (PTB7) and [6,6]-phenyl-C71-butyric acid methyl ester (PC71BM) is studied. Different alcohols are tested and besides the most commonly used methanol treatment, other alcohols such as ethanol, 2-propanol, and 1-butanol also improve the device performance as compared to untreated solar cells. Changes of the surface structure caused by the alcohol treatment are probed with AFM and the modification of inner film morphology is probed by time of flight-grazing incidence small angle neutron scattering (TOF-GISANS). UV/Vis measurements show that the thickness of all BHJ films remains unchanged by the different solvent treatments. Thus, the enhanced device performance induced by the alcohol treatments is correlated to the reconstruction of the inner film structures probed with TOF-GISANS and the modified energy levels at the interfaces between the BHJ layer and the aluminum electrodes, evident by the enhanced short-circuit current and open-circuit voltage of the I-V curves.

CPP 36.11 Wed 12:15 C 130

**Control of Structural Order and Phase Separation in Polymer-Fullerene Solar Cells** — •Christian Kästner[1], Daniel A. M. Egbe[2], and Harald Hoppe[1] — [1]Institute of Physics, Technische Universität Ilmenau, Ilmenau, Germany — [2]Linz Institute for Organic Solar Cells, Johannes Kepler University, Linz, Austria

It is common knowledge that polymer aggregation and phase separation in blends with fullerene derivatives is a delicate issue and crucially impacts the photovoltaic parameters of polymer based solar cells. On the one side, strongly intermixed polymer:fullerene phases provide large interfacial area and consequently large exciton dissociation rates and thus charge carrier generation. On the other side, pristine, and eligibly ordered, polymer or fullerene domains support exciton delocalization and efficient charge transport. Herein, we present versatile routes to control the morphology by applying side-chain modifications to the polymer and fullerene, tuning the polymer:fullerene blend ratio and controlling the order within the bulk heterojunction via ternary blends. On the basis of an anthracene-containing poly(p-phenylene-ethynylene)-alt-poly(p-phenylene-vinylene) (PPE-PPV) copolymer backbone we investigated a number of these structure-property-relations. As an imposing result it is demonstrated that via manipulation of molecular structure and processing parameters enables tuning bulk morphologies at will.

CPP 36.12 Wed 12:30 C 130

**Influence of post-production thermal stress on organic photovoltaic cells** — •Arne Hendel, Marlis Ortel, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

One of the mayor challenges of organic photovoltaic cells towards large scale industrial production is the lifetime of the organic solar cells. Accelerated lifetime tests can be performed by applying thermal stress to the devices. In this study, PTB7:PCBM bulk hetero-junction solar cells were exposed in a post-production thermal heat step to temperatures up to 140°C. The reaction to thermal stress was investigated by impedance analysis and light intensity dependent I-V characteristics. It was found that the overall conductivity improved by thermal stress. In addition, an asymmetric series resistance which depends strongly on the light intensity was found by the light intensity dependent measurements. Furthermore, an investigation of the diode characteristic in dark revealed a deterioration of the blocking behaviour for reverse voltages. The results of the impedance analysis and light intensity dependent measurements were compared to AM1.5G I-V characterization, which was used to monitor the degradation of the device performance. A physical device model including the contact properties of the solar cells is presented to explain the findings.

CPP 36.13 Wed 12:45 C 130

**How intrinsic photo-degradation impacts photovoltaic device performance in organic solar cells** — •Thomas Heumueller[1], Timothy Burke[2], William Mateker[2], Michael McGehee[2], and Christoph Brabec[1,3] — [1]Universität Erlangen-Nürnberg — [2]Stanford University — [3]ZAE Bayern

As organic PV efficiencies exceed 10%, the science of stabilization and lifetime gains importance. Several degradation phenomena in organic solar cells are related to an increase in trap density, but the mechanisms of how different types of traps affect open-circuit voltage, short-circuit current and fill factor need considerably more investigation. To separate effects from several different degradation mechanisms that usually occur at the same time, we perform tests under controlled environmental conditions and distinguish between bulk and interface effects by de-laminating and replacing electrodes. Interfacial degradation is observed to predominantly affect the fill factor, most likely due to the formation of energetic barriers and can be reversed by reapplying new electrodes. Bulk degradation in amorphous systems, like PCDTBT, results in a loss of open circuit voltage. Using charge extraction and transient photovoltage we show that the Voc losses are not caused by increased recombination, but rather by a broadening in the density of states. Crystalline materials demonstrate an increased stability against Voc losses, most likely due to a high charge carrier density at Voc. Sometimes a characteristic loss of short circuit current is observed in crystalline materials. We show that those losses can be prevented by choosing a different acceptor material.

## CPP 37: Interfaces and Thin Films III (joint session CPP, DS)

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

CPP 37.1 Wed 9:30 C 243

**Patterned Diblock co-polymer Thin Films as Templates for Advanced Anisotropic Metal Nanostructures** — •Stephan V. Roth[1], Gonzalo Santoro[1], Johannes F.H. Risch[1], Shun Yu[2], Matthias Schwartzkopf[1], Peng Zhang[1], Sarathlal Koyiloth Vayalil[1], Michael A. Rübhausen[3], Nick J. Terrill[4], Paul Staniec[4], Yuan Yao[5], Ezzeldin Metwalli[5], and Peter Müller-Buschbaum[5] — [1]DESY, Notkestr. 85, 22607 Hamburg — [2]KTH, Teknikringen 56-58, 10044 Stockholm — [3]Inst. f. Nanostruktur- und Festkörperforschung, CFEL, APOG, Univ. Hamburg, Luruper Chaussee 149, 22761 Hamburg — [4]DLS, Harwell Sci. & Innov. Campus, Didcot, Oxfordshire OX11 0QX — [5]LS funkt. Mat., Physik-Department, TU München, James-Franck-Str. 1, 85748 Garching

The tailoring of the metal-polymer interface in hybrid materials plays a crucial role in modern advanced material science. Using glancing angle deposition of gold on a nanostructured diblock copolymer thin film (PS-b-PMMA), we are able to fabricate directional hierarchical structures. This approach exploits the selective wetting of Au on the PS block. We prove the asymmetric, localized growth of the gold nanoparticles and are able to extract the different growth laws by in situ scattering methods as well as imaging methods. The optical anisotropy of these hierarchical hybrid materials is probed by angular resolved spectroscopic methods and is correlated to the nanostructure. This approach offers the possibility to tailor functional hierarchical thin films for plasmonics and metamaterials, as nanoantennae arrays, in organic photovoltaics and sensor electronics.

CPP 37.2 Wed 9:45 C 243

**Transparent aluminium oxide coatings on polymer substrate** — •Samantha Micciulla[1], Xiaofei Duan[2], Robert N. Lamb[2], and Regine von Klitzing[1] — [1]Technische Universitaet Berlin — [2]The University of Melbourne

Smart coatings are highly versatile systems, applicable to diverse purposes and finely tunable by proper external stimuli. Polymers are mostly used to create responsive films, however they suffer hard conditions like high temperatures, aggressive chemicals, high mechanical stress, with consequent degradation or irreversible modifications. Therefore the use of a thin inorganic coating enriching the system of high mechanical and chemical stability may be the solution to this limitation. A good candidate to this purpose is aluminium oxide ($Al_2O_3$), which presents anti-corrosion properties, high wear resistance, and high biocompatibility. Moreover, the transparency of alumina ceramics in the UV-Vis range makes it suitable to optical applications. A synthetic route to prepare $Al_2O_3$ was developed to reduce the risk of degradation of the underneath polymer, using low temperatures and mild chemicals. The composition of alumina/polymer coatings was studied by X-Rays Photoelectron Spectroscopy and the surface morphology by Scanning Electron Miscoscopy. The latter showed the achievement of a smooth, cracks-free coating upon hydrothermal treatment (105°C, 38 atm). Our studies focused on the preparation of alumina coatings on polymer substrates having different surface hydrophilicity, charge and structure, and revealed that the wetting properties of the polymer surface play the dominant role for the quality of the coating.

CPP 37.3 Wed 10:00 C 243

**Tailoring the mechanics of ultrathin carbon nanomembranes by molecular design** — •Xianghui Zhang, Christof Neumann, Polina Angelova, André Beyer, and Armin Gölzhäuser — Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany

Freestanding carbon nanomembranes (CNMs) with a thickness between 0.6 nm and 1.7 nm were prepared from self-assembled monolayers (SAMs) of diverse polyaromatic precursors via low energy electron induced cross-linking. The mechanical properties of CNMs were investigated by applying a pressure difference between the two sides of the membrane and by measuring the resulting deflection with atomic force microscopy. We found a correlation between the rigidity of the precursor molecules and the macroscopic mechanical stiffness of CNMs. While CNMs from rigid and condensed precursors like naphthalene and pyrene thiols prove to exhibit higher Young's moduli of 15~19 GPa, CNMs from non-fused oligophenyls possess lower Young's moduli of ~10 GPa. For CNMs from less densely packed SAMs, the presence of defects and nanopores plays an important role in determining their mechanical properties. The finite element method (FEM) was applied to examine the deformation profiles and simulate the pressure-deflection relationships.

CPP 37.4 Wed 10:15 C 243

**Covalent modification of large area monolayer graphene towards biosensing.** — •Felix Rösicke[1], Marc Gluba[1], Guoguang Sun[2], Karsten Hinrichs[2], Jörg Rappich[1], and Norbert Nickel[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]Leibniz - Institut für Analytische Wissenschaften - ISAS - e.V., Department Berlin, Berlin, Germany

We investigated the electrochemical grafting of para-N-maleimidophenyl (pMP) onto graphene from the respective diazonium salt (p-(N-Maleimido)benzenediazonium tetrafluoroborate, pMPDT) by electrochemical quartz crystal microbalance (EQCM), Raman- and infrared spectroscopies.

The p-MP is well known to react with any SH-group present in solution and is therefore a possible candidate to build up bio-sensing devices which, in combination with graphene, are very stable and conductive systems that can be transferred to any substrate. The sample preparation was performed by a transfer of CVD grown large area graphene [1] to an isolating layer of SiNx on Au-coated QCM chips. Using graphene as working electrode, the current behavior and the change in the resonant frequency of the EQCM reflect the electrochemical reduction of the diazonium compound. Raman and infrared spectroscopies reveal the binding of pMP onto the graphene layer. The charge used for the reduction of pMPDT correlates to the amount of grafted pMP and the observed defect density of graphene. Finally the pMP functionalized graphene surface was tested by reaction with 4-Nitrobenzenethiol.

CPP 37.5 Wed 10:30 C 243

**Light absorption of Ultrathin Gallium Layers during Oxidation** — •Frank Lawrenz[1], Chrisitane A. Helm[1], and Stephan Block[2] — [1]Physik, Uni Greifswald, 17487 Greifswald, Germany — [2]Chalmers University of Technology, 412 96 Göteborg, Sweden

The fabrication of ultrathin metal oxide layers is important for many technological applications. Here we describe a simple method for the formation of 3 nm thick gallium oxide layers which extent up to 1 cm2. Liquid gallium is applied onto silica surfaces, leaving thin layers that are immediately oxidized at their surface under ambient conditions, followed by slower oxidation of the remaining layer. This is quantified using UV-Vis absorption measurements, indicating that the oxidation of the entire layer is completed after two weeks. A rate model is developed to describe the oxidation of ultrathin Ga layers.

CPP 37.6 Wed 10:45 C 243

**Ambiguous Copolymer Surfaces from Light-Mediated Radical Polymerization** — •Christian W. Pester[1,2], Justin E. Poelma[2], Craig J. Hawker[2], and Edward J. Kramer[1] — [1]UC Santa Barbara, Department of Materials, Department of Chemical Engineering — [2]Department of Chemistry and Biochemistry, Materials Research Laboratory, Santa Barbara, CA, 93106

We describe the use of visible-light-mediated living radical polymerization of methacrylate-based, anti-fouling relevant monomers, i.e., poly(trifluoroethyl methacrylate) (TFEMA) and poly(ethylene glycol methacrylate) (PEGMA). Resulting ambiguous surfaces are expected to show promising features for marine anti-fouling applications. Light-catalysis affords facile lithographic patterning. In this PEGMA-b-TFEMA case study we patterned these diblocks to give topographically and chemically well-defined ambiguous surfaces which combine hydrophilic and hydrophobic properties on the micron length scale. XPS, dynamic secondary ion mass spectroscopy, and scanning x-ray transmission microscopy, allowed us to precisely determine chemical surface composition, whereas AFM afforded precise analysis of topographical features inherent to patterning. The light-activated polymerization method we use was readily coupled to well-established ATRP techniques and afforded expansion of this case study to advanced monomers, e.g, highly fluorinated compounds and zwitterionic acrylates. Polymer backbone functionalization combined with lithography allowed spatial control over brush architecture, adding to the wide chemical and conformational accessible parameter space.

**15 min. break**

CPP 37.7 Wed 11:15 C 243

**Light-Controlled Molecular Zippers based on Azobenzene Main Chain Polymers** — •Christopher Weber[1], Tobias Liebig[1], Anton Zykov[1], Linus Pithan[1], Sebastian Bommel[1,2], David Bléger[3], and Stefan Kowarik[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin — [2]Deutsches Elektronen-Synchrotron, 22607 Hamburg — [3]Institut für Chemie, Humboldt-Universität zu Berlin, 12489 Berlin

We report that thin films of azobenzene main chain polymers with interdigitating dodecyl side chains (molecular zippers) can be switched reversibly with light between a semicrystalline and an amorphous state, corresponding to a closed and open state of the molecular zippers. Simultaneous time-resolved x-ray diffraction and optical spectroscopy measurements show that the kinetics of the amorphization of the crystalline domains is about 12 times slower than the photoisomerization of the azobenzene chromophores. Our findings suggest that the amorphization is triggered by *E-Z* isomerization of a small amount of azobenzene chromophores within the polymer film and that the slower kinetics of the photoinduced amorphization is determined by structural and topological constraints and not by a different isomerization mechanism in crystalline domains.

CPP 37.8 Wed 11:30 C 243

**Monte Carlo Simulations for Switchable Model Molecules** — •Raffaele Tavarone[1], Patrick Charbonneau[2], and Holger Stark[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Departments of Chemistry and Physics, Duke University, Durham, North Carolina 27708, USA

Light-switchable molecules are chemical compounds that can undergo a light-induced, reversible *trans-cis* isomerization. They can be used to build functional monolayers with, for example, switchable wetting properties. A typical example of a light-driven *trans-cis* transition is the azobenzene isomerization.

Inspired by the conformational changes of the azobenzene compound, we build a model in which a *trans* isomer is regarded as a straight needle while a *cis* isomer is regarded as a bent needle. First, we determine the phase behavior of such molecules on a planar surface using Monte Carlo simulations. The resulting phase diagram (density versus molecular shape) shows several liquid-crystal mesophases.

Second, we build a kinetic model for a glassy monolayer inspired by a recent experiment [1]. They showed that the spontaneous algebraic relaxation of orientational order, inscribed in the sample with linearly polarized light, is strongly enhanced by illumination with circularly polarized light. In our simulations we allow molecules to switch between the *trans* and *cis* isomers due to the interaction with light. We are able to trace the influence of neighbors hindrance and other microscopic processes on the kinetic of the relaxation reported in the experiment.

[1] Fang, G. J., et al., Nature communications **4**, 1521 (2013).

CPP 37.9 Wed 11:45 C 243

**Effect of Binary Polymer Mixtures on the Growth of Polyelectrolyte Multilayers** — •Malte Passvogel, Peter Nestler, and Christiane A. Helm — Physik, Uni Greifswald, 17487 Greifswald, Germany

The buildup of polyelectrolyte multilayers (PEMs) is investigated in solution with multiple angle null-ellipsometry. Polyanion poly(styrenesulfonate) (PSS) and polycation polydiallyldimethylammonium (PDADMAC) are adsorbed sequentially from 0.1 NaCl solution. After $N_{trans}$ deposited PDADMAC/PSS layer pairs a transition from parabolic to linear growth occurs, then the thickness per layer pair $d_{BL}$ is constant. $d_{BL}$ is 12.3 nm, if the molecular weight ($M_w$) exceed threshold values which are specific for each polymer (25 kDa for PSS and 80 kDa for PDADMAC). If either the PDADMAC or the PSS molecular weight is decreased below the threshold values, $d_{BL}$ either falls (for PDADMAC) or rises (for PSS) suggesting very different growth modes. Binary mixtures of PDADMAC and PSS with $M_w$ below and above the threshold value are used, while $M_w$ of the complementary polyion is kept above the threshold. $d_{BL}$ depends linearly on the mole fraction of the low-molecular-weight PDADMAC. However, $d_{BL}$ is only influenced by low-molecular-weight PSS, if its molar fraction exceeds 90%. Always, the same linear relationship between $N_{trans}$ and $d_{BL}$ is found. These observations can be explained with an asymmetric growth model of polyelectrolyte multilayers.

CPP 37.10 Wed 12:00 C 243

**The Swelling Behaviour of Voids inside Polyelectrolyte Multilayers** — •Maximilian Zerball[1], Ralf Köhler[2], Olaf Soltwedel[3], and Regine von Klitzing[1] — [1]Institut für Chemie, Technische Universität Berlin, Str. 17.Juni 124, 10623 Berlin — [2]Institut für Weiche Materie und funktionelle Materialien, Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, 14109 Berlin — [3]Max-Planck-Institut für Festkörperforschung, Lichtenbergstr. 1, 85747 Garching

Polyelectrolyte Multilayer (PEM) are organic films built up via subsequent adsorption of oppositely charged polyions. PEMs are highly sensitive to external parameter like the relative humidity (r.h.) of the ambient atmosphere. This ability makes them to ideal candidates for sensoric applications. In order to use these films as sensors it is important to understand and to control the swelling behavior. The uptaken water of swollen PEMs are subdividable into two contributions; the swelling water, which influences thickness and optical properties, and the void water, which only affects the optical properties of the PEM.

The swelling behavior of voids, i.e. the separated amount of uptaken water inside voids in comparison to the uptaken amount of water inside the PEM with increasing r.h., is rarely researched. For the purpose to understand the swelling behavior of voids more in detail, in this study the void water and swelling water of PEMs in dependence of the relative humidty was investigated by neutron reflectivity. The results suggest that the strongest increase of voidwater proceeds between 0% r,h, and 6% r.h. while beyond, the swelling water dominates the amount of water.

CPP 37.11 Wed 12:15 C 243

**Influence of Barrier Layers on Interdiffusion in Polyelectrolyte Multilayers** — •Peter Nestler[1], Malte Passvogel[1], Olaf Soltwedel[2], Ralf Köhler[3], and Chrisitane A. Helm[1] — [1]Physik, Uni Greifswald, 17487 Greifswald, Germany — [2]MPI FKP 70569 Stuttgart, Germany — [3]Helmholtz-Zentrum Berlin, 14109 Berlin, Germany

Polyelectrolyte multilayers are made from poly(diallyldimethylammonium) (PDADMA), poly(styrenesulfonate) (PSS). Using selective PSS deuteration each film consists of a protonated and a deuterated compartment.

During annealing in 1 M NaCl solution the internal interface between these two compartments broadens due to interdiffusion. The PSS diffusion coefficient $D_{PSS}$ inside the multilayer film is quantified via neutron reflectivity. Eventually the annealing leads to a uniform distribution of protonated and deuterated PSS inside the film. If one polycation layer in the film centre is branched poly(ethyleneimine) (PEI), then PEI serves as a diffusion barrier. In this case the barrier is impenetrable for up to 70% of PSS molecules. The diffusion behaviour of the remaining 30% can be described using a position-dependent distribution of DPSS inside the multilayer film. The effective PSS diffusion coefficient is reduced by one to two orders of magnitude.

CPP 37.12 Wed 12:30 C 243

**Improved Electrolyte-Additive Induced Performance of Graphite Anodes for Lithium-Ion Batteries – Electrochemical and Electrode Surface Studies** — •Anna Dimitrova[1], Andre Müller[2], Svetlozar Ivanov[2], Marcel Himmerlich[1], Anja Eisenhardt[1], Andreas Bund[2], and Stefan Krischok[1] — [1]Technische Universität Ilmenau, Institut für Physik and Institut für Mikro- und Nanotechnologien, Germany — [2]Technische Universität Ilmenau, Fachgebiet Elektrochemie und Galvanotechnik, Germany

The electrolyte decomposition is a crucial stage in the formation cycle of Li–ion batteries. It results in the formation of a protective passivation layer on the graphite electrode surface, called *solid electrolyte interphase* (SEI). SEI formation competes with Li ion incretion and its chemical composition and structure determines the battery cell life time. To control this process we designed a phosphorous enriched electrolyte, which enhances the rate performance and the capacity retention of the Li–ion battery compared to a non-modified electrolyte. In order to study charge-discharge cycles in the batteries and to analyze the SEI composition, we combined electrochemical studies with X-ray Photoelectron Spectroscopy (XPS). In this work the influence of the electrolyte on the SEI composition was investigated and a correlation between chemical structure and electrochemical characteristics of the Li–ion battery will be discussed.

CPP 37.13 Wed 12:45 C 243

**Deposition of copper multilayers on Au(111) in sulphuric acid solution: An electrochemical scanning tunneling microscopy study** — •Bartosz Madry[1], Klaus Wandelt[1,2], and Marek Nowicki[1] — [1]Institute of Experimental Physics, University of Wroclaw, pl. M. Borna 9, 50-204 Wroclaw, Poland. — [2]Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, 53115 Bonn, Germany.

The co-adsorption of submono-, mono- and multi-layers of Cu with sulfate anions on a Au(111) electrode surface was investigated in electrochemical environment (0.1 mM $CuSO_4$ + 0.1 M $H_2SO_4$) by cyclic voltammetry (CV) and in-situ scanning tunneling microscopy (STM). Correlated with the STM investigations the CV measurements indicate co-adsorption/-desorption processes of Cu of submono-, mono- and multi-layer coverages with sulfuric acid species on Au(111). The formation of a quasi-hexagonal Moiré superstructure on terraces of copper multilayers was observed in situ by STM. In detail the observed Moiré-structure is similar but not identical to the one observed on the (111) surface of bulk copper. High resolution STM images show the formation of a $(\sqrt{3}\times\sqrt{7})$ -like sulfate structure on all multilayer copper terraces.

## CPP 38: Computational Physics of Soft Matter I

Time: Wednesday 9:30–13:00 Location: C 264

**Invited Talk** CPP 38.1 Wed 9:30 C 264

**Challenges for the development of coarse-grained simulation models for complex soft matter systems** — •Christine Peter — University of Konstanz, Germany

Inherent to the concept of coarse graining is a loss of transferability, i.e. a decreasing ability to correctly describe a system at several thermodynamic state points. Intimately linked to this is a loss of the ability to correctly represent all structural, thermodynamic and dynamic properties of the system. Examples for these limitations are easily found in all coarse-grained (CG) simulations of multicomponent or multiphase soft matter systems. Here, one needs to solve the question how to represent phase transitions, phase coexistence, conformational transitions that are coupled to environmental changes, surface effects, etc. This is not only connected to finding an appropriate method of generating CG potentials but also to understanding one's choice of reference state point. On top of these thermodynamic challenges, one needs to be aware of the problem of dynamics in CG models: coarse graining leads to accelerated dynamics due to smoother (free) energy landscapes compared to higher-resolution descriptions. Approaches to rigorously map dynamics of models on different scales are limited to simple model systems, while in soft matter systems different dynamic processes may experience different speedups – a challenge for a correct representation of pathways and intermediates. I will use a liquid crystalline as well as biomolecular systems as examples to illustrate the above aspects of CG simulation models.

CPP 38.2 Wed 10:00 C 264

**Thermodynamic and microscopic aspects of cosolvent-specific effects in coil-to-globule transition** — •Jan Heyda[1] and Joachim Dzubiella[2,3] — [1]Department of Physical Chemistry, Institute of Chemical Technology, Prague, Czech Republic — [2]Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, Germany — [3]Department of Physics, Humboldt-University Berlin, Germany

An implicit-solvent, explicit-cosolvent Langevin dynamics of generic homopolymer provides three distinct regimes of cosolvent effects on coil-to-globule transition; namely cosolvent exclusion, weak binding, and strong binding, i.e., bridging (10.1021/ma302320y). We have introduced thermodynamic model interpreting observed regimes of cosolvent effects on the cloud-point temperatures of thermoresponsive polymers (10.1021/jp5041635). The microscopic details (excess adsorptions) from solution theory are approachable by simulation methods.

Original study was thus extended for an effect of cosolvent concentration. Results are in accord with our thermodynamic model and provide a consistent framework for cosolvent effects on cloud-point temperature. Among others, transition entropy was found to be independent of, or weakly, and strongly decreasing with cosolvent concentration in three regimes. All, in accord with recent calorimetry data.

Interpretation of protein denaturation/stability data is a next application of our model, which moreover accounts for and interpret reentrant transition (coil-globule-coil), grabbing recently experimental and theoretical attention (dx.doi.org/10.1038/ncomms5882).

CPP 38.3 Wed 10:15 C 264

**Relative resolution: A hybrid strategy for molecular modeling** — •Aviel Chaimovich[1], Kurt Kremer[1], and Christine Peter[2] — [1]Max-Planck-Institut für Polymerforschung, Mainz — [2]University of Konstanz, Konstanz

Over the past decade, hybrid strategies, which switch from a full-atomistic (FA) to a coarse-grained (CG) description in terms of a spatial coordinate, have become numerous [1-4]. Concurrently, parametrization procedures, which aim at generating an optimal CG model given a reference FA model, have also become common [5]. In this work, we develop a hybrid strategy which naturally attains a very efficient parametrization scheme. Our approach appears to be especially powerful for modeling multi-component mixtures.

[1] M. Praprotnik, L. Delle Site, and K. Kremer. The Journal of Chemical Physics, 123(22):224106, 2005.

[2] C. F. Abrams. The Journal of Chemical Physics, 123(23):234101, 2005.

[3] B. Ensing et al. Journal of Chemical Theory and Computation, 3(3):1100-1105, 2007.

[4] R. Potestio et al. Physical Review Letters, 110(10):108301, 2013.

[5] W. G. Noid. The Journal of Chemical Physics, 139(9):090901, 2013.

CPP 38.4 Wed 10:30 C 264

**The role of stiffness in polymer aggregation: Leading from amorphous aggregates to polymer bundles** — •Johannes Zierenberg and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Germany

We use parallel multicanonical simulations of a few homopolymers in order to map out generic temperature-stiffness structural phase diagrams, from flexible to stiff polymers. The systematic overview highlights the key role of stiffness on structural phases in polymer aggregation for an entire class of semiflexible polymers covering both the limit of flexible theta polymers and the worm-like chain limit. The structural motifs range from amorphous aggregates to twisted polymer bundles, for rather flexible and rather stiff polymers respectively. For the first-order aggregation transition of several polymers, we provide strong evidence that the free-energy barrier increases with stiffness. Thus, this general study of an entire class of semiflexible polymers supports recent claims that the free-energy barrier for the transition into bundles is larger than for the transition into amorphous aggregates.

CPP 38.5 Wed 10:45 C 264

**Aggregation of flexible polymers under spherical constraints** — Johannes Zierenberg, •Marco Mueller, Philipp Schierz, Martin Marenz, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Germany

Applying parallel multicanonical simulations, we study the aggregation transition of finite flexible polymers in dependence on the density, where we keep the polymer length fixed as a chemical property. A spherical confinement is imposed to control the translational entropy. We show that the competition between single-polymer collapse and many-polymer aggregation yields a lower temperature bound for the isolated chain approximation. For dilute polymers, we present entropic and energetic arguments that allow to relate the inverse aggregation to the density of the monodisperse systems.

**15 min. break.**

CPP 38.6 Wed 11:15 C 264

**Conformations of a Long Polymer in a Melt of Shorter Chains: Generalizations of the Flory Theorem** — •Michael Lang[1], Michael Rubinstein[2], and Jens-Uwe Sommer[1,3] — [1]Leibniz Institute of Polymer Research Dresden, Hohe Straße 6, 01069 Dresden, Germany. — [2]Department of Chemistry, University of North Carolina, Chapel Hill, North Carolina 27599-3290, United States. — [3]Institute of Theoretical Physics, Technische Universität Dresden, Zellescher Weg 17, 01062 Dresden, Germany.

Large scale simulations of the swelling of a long $N$-mer in a melt of chemically identical $P$-mers are used to investigate a discrepancy between theory and experiments. Classical theory predicts an increase of probe chain size $R \sim P^{-0.18}$ with decreasing degree of polymerization $P$ of melt chains in the range of $1 < P < N^{1/2}$. But both experiment and simulation data are more consistent with an apparently slower swelling $R \sim P^{-0.1}$ over a wider range of melt degrees of polymerization. This anomaly is explained by taking into account the recently discovered long range bond correlations in polymer melts and corrections to excluded volume. We generalize the Flory theorem and demonstrate that it is in excellent agreement with experiments and simulations.

CPP 38.7 Wed 11:30 C 264

**Lattice Monte Carlo simulations of polymer melts** — •Hsiao-ping Hsu — Max-Planck-Institut für Polymerforschung, Mainz, Germany

We use Monte Carlo simulations to study polymer melts consisting of fully flexible and moderately stiff chains in the bond fluctuation model at a volume fraction 0.5. In order to reduce the local density fluctuations, we test a pre-packing process for the preparation of the initial configurations of the polymer melts, before the excluded volume interaction is switched on completely. This process leads to a significantly faster decrease of the number of overlapping monomers on the lattice. It is useful for studying the statistical properties of the model with a marginally incomplete elimination of excluded volume violations. We find that the internal mean square end-to-end distance for moderately stiff chains in a melt can be very well described by a freely rotating chain model with a precise estimate of the bond-bond orientational correlation between two successive bond vectors in equilibrium. The plot of the probability distributions of the reduced end-to-end distance of chains of different stiffness also shows that the data collapse is excellent and described very well by the Gaussian distribution for ideal chains. However, while our results confirm the systematic deviations between Gaussian statistics for the chain structure factor for fully flexible chains in a melt, we show that for the available chain length these deviations are no longer visible, when the chain stiffness is included. The mean square bond length and the compressibility estimated from collective structure factors

**Invited Talk** CPP 38.8 Wed 11:45 C 264

**Answering old questions with new simulation methods: what is the behavior of fluctuation spectra and Frank constants in polymer nematics?** — •Kostas Daoulas and Patrick Gemünden — Max-Planck-Institut für Polymerforschung, Mainz, Germany

Long wavelength behavior of dense polymer nematics has attracted considerable attention from the physics community due to intriguing features. In contrast to liquid crystals (LC) with small molecules, linking mesogenes into polymer chains leads to long-range coupling of density and director fluctuations. Thus related correlation functions exhibit unusual behavior, the "bowtie shape" of the density structure factor being a characteristic example. Several analytical theories have been developed, describing fluctuation spectra and related elastic constants (e.g. Frank constants). Interestingly, some of the theoretical results are very controversial. The growth of the splay constant with chain length is a well-known example, where linear (Meyer, 1982) and quadratic (de Gennes, 1982) dependencies were predicted.

In this study we validate early analytical theories employing efficient Monte Carlo simulations of polymer nematics described by a worm-like chain model combined with soft anisotropic non-bonded interactions. We demonstrate that the analytical theories indeed can capture several features of the fluctuation spectra calculated from simulation data. Based on these spectra, elastic constants are extracted and compared with theoretical predictions. Our results are found to support strongly the theories proposing a linear dependence of splay constant on chain length.

CPP 38.9 Wed 12:15 C 264

**Molecular Dynamics Simulations of Hyperbranched PAMAM Vicsek Fractals** — •Florian Fürstenberg[1], Andrey A. Gurtovenko[2], Maxim Dolgushev[1], and Alexander Blumen[1] — [1]Theoretische Polymerphysik, Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Deutschland — [2]Institute of Macromolecular Compounds, Russian Academy of Sciences, Bolshoi pr. V.O. 31, St. Petersburg, 199004 Russia

In the last few years hyperbranched macromolecular structures have become an important field of investigation. Within this broad class, highly symmetrical polymers (such as dendrimers) are of special theoretical interest. While dendrimers were extensively synthesized, Vicsek fractals (VF) constitute another interesting class of symmetrical, deterministic structures. Here we introduce the new class of polyamidoamine Vicsek fractals (PVF). Although a VF architecture is not being synthesized so far, we study PVF *in silico* and employ extensive molecular dynamics simulations along with the coarse-grained MARTINI force-field[1] to unravel their structural and dynamic characteristics in dilute solution. Following the method developed for PAMAM dendrimers (PD) in Ref. [2], allows us to discuss the differences in the investigated quantities for PD and PVF brought about by their different molecular architectures[3].

[1] S.J. Marrink et al., J. Phys. Chem. B 27, 7812 (2007).
[2] H. Lee and R.G. Larson, Macromolecules 44, 2291 (2011).
[3] F. Fürstenberg et al., Macromol. Theory Simul. (2014). DOI: 10.1002/mats.201400063

CPP 38.10 Wed 12:30 C 264

**Collective Motion of Spherical Microswimmers in a Quasi-2D Geometry** — •Maurice Maurer, Andreas Zöttl, and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin

The collective motion of microorganisms and artificial microswimmers exhibits interesting dynamic structure formation on length scales much larger than the size of an individual particle.

Experiments with self-propelled colloids in a quasi-2D geometry show dynamic clustering behavior and phase separation due to hydrodynamic interactions. Motivated by these experiments, we numerically investigate the collective behavior of spherical model swimmers [1]. Using domain decomposition and the message passing interface (MPI), we developed a highly scalable parallel version of multi-particle collision dynamics - a particle-based solver of the Navier-Stokes equations.

Here we study squirmers, which mimic the propulsion mechanism of active emulsion droplets and ciliated microorganisms like volvox algae by a surface velocity field. Furthermore, we simulate active Janus particles, the surfaces of which are only partly active. For low densities the colloids show gas-like behavior while at high densities crystalline structures emerge. Only for neutral squirmers and Janus particles almost fully covered by the active region, we observe that structural order increases steeply at a critical density, indicating a non-equilibrium phase transition. Finally, we also show how system size and reducing the colloidal degrees of freedom influence our findings.

[1] A. Zöttl and H. Stark, Phys. Rev. Lett. 112, 118101 (2014).

CPP 38.11 Wed 12:45 C 264

**Interactions at the solid-liquid interface from a molecular simulation perspective** — •Peter Spijker[1], Bernhard

Reischl[2], and Adam Foster[1] — [1]COMP Centre of Excellence, Department of Applied Physics, Aalto University, Helsinki, Finland — [2]Nanochemistry Research Institute, Curtin University, Perth, Australia

Solid-liquid interfaces are ubiquitous and have an important, if not fundamental, role in many phenomena from different fields. But despite the importance of these interfaces, deep understanding of the physical properties of them remains scarce. Atomic force microscopy (AFM) has the advantage of probing the solid-liquid system locally and it allows sub-nanometer studying of the interface. Combined with large-scale molecular dynamics (MD) simulations we are able to start to elucidate the physical origins of the solid-liquid interfaces. Over the last few years considerable experimental and theoretical progress has been made in understanding the water hydration structure on different atomically flat surfaces. In the current work we show how MD simulations and theoretical analysis can be used to understand much more complex hydration structures on non-trivial solid-liquid interfaces (molecular crystals, clay surfaces, etc.) and to allow for as direct comparison as possible between theory and experiment. In the case of the calcite-water interface we modeled the AFM tip and are capable to extract force curves similar to experimental data. Our joined theoretical and experimental approach demonstrates our ability understanding details of these heterogeneous molecular solid-liquid interfaces.

## CPP 39: Cell adhesion, mechanics and migration I (Joint session BP, CPP)

Time: Wednesday 9:30–13:15 Location: H 1058

**Invited Talk** CPP 39.1 Wed 9:30 H 1058

**Feeling for cell function: Mechanical phenotyping at 100 cells/sec** — •Jochen Guck — Technische Universität Dresden, Germany

The mechanical properties of cells have long been heralded as a label-free, inherent marker of biological function in health and disease. Wide-spread utilization has so far been impeded by the lack of a convenient measurement technique with sufficient throughput. To address this need, we introduce real-time deformability cytometry (RT-DC) for the continuous mechanical single-cell characterization of large populations ($>$ 100.000 cells) with analysis rates greater than 100 cells/s, approaching that of conventional fluorescence-based flow cytometers. Using RT-DC we can sensitively detect cytoskeletal alterations, distinguish cell cycle phases, track hematopoietic stem cell differentiation into distinct lineages and characterize cell*populations in whole blood by their mechanical fingerprint. Our results indicate that cell mechanics can define cell function, can be used as an inherent cell marker and could serve as target for novel therapies. Mechanical phenotyping adds a new functional, marker-free dimension to flow cytometry with diverse applications in biology, biotechnology and medicine.

CPP 39.2 Wed 10:00 H 1058

**Characterizing viscoelastic properties of the cortex in mitotic cells** — •Elisabeth Fischer-Friedrich[1,2], Jonne Helenius[3], Anthony Hyman[2], Daniel Müller[3], and Frank Jülicher[1] — [1]MPI PKS, Nöthnitzerstr. 38, 01187 Dresden, Germany — [2]MPI CBG, Pfotenhauerstr. 108, 01307 Dresden, Germany — [3]D-BSSE, ETHZ, Mattenstr. 26, 4058 Basel, Switzerland

Cell stiffness is a key parameter for our understanding of cell shape, cell migration and tissue organization. However, as the cell consists of several components, it is challenging to extract the force contribution and the elastic modulus of a specific component upon cell deformation. Here, we probe the stiffness of round, mitotic HeLa cells in a parallel plate compression setup, where we measure the force necessary to compress cells in between plates. An earlier study showed that in steady state, this force is due to cell surface tension. Here, we apply step strains and sinusoidal modulation of the plate distance at various frequencies allowing us to probe differential cell stiffness. We find strong indications that cell stiffness in mitosis is dominated by actomyosin and therefore by the mitotic cortex. This interpretation allows to extract an associated frequency-dependent area extension modulus. We show that myosin activity at the same time fluidizes and stiffens cells, where differential cell stiffness increases linearly in dependence of active prestress. On the other hand, the passive cross-linker $\alpha$-actinin solidifies and stiffens mitotic cells. Our study shows how active and passive cross-linkers influence rheological properties of the cortical actin-network in vivo.

CPP 39.3 Wed 10:15 H 1058

**Biogenic cracks in porous medium** — •Arnaud Hemmerle[1], Jörn Hartung[1], Oskar Hallatschek[1,2], Lucas Goehring[1], and Stephan Herminghaus[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — [2]Department of Physics, University of California, Berkeley, CA, USA

Microorganisms growing on and inside porous rock may fracture it by various processes. Most of the studies have been on the chemical aspects of biofouling and bioweathering, while mechanical contributions have been neglected. However, as witnessed by the perseverance of a seed germinating and cracking up a concrete block, the turgor pressure of living organisms can be very significant. It is the effects of such mechanical forces on the weathering of porous media that will concern us here. We designed a model porous medium made of glass beads held together by polydimethylsiloxane (PDMS) capillary bridges. The rheological properties of this material can be controlled by the curing conditions and the crosslinking of the PDMS. Glass and PDMS being inert to most chemicals, we are able to focus on the mechanical processes of biodeterioration, excluding any chemical weathering.

Inspired by recent measurements of the high pressure ($\simeq$0.5 Mpa) exerted by a growing population of yeast trapped in a microfluidic device, we show that yeast cells can be cultured homogeneously within porous medium and investigate then the effects of such an inner pressure on the mechanical properties of the sample. We observe crack propagation for a certain range of bead sizes and cohesiveness, showing a clear interaction between biotic and abiotic processes.

CPP 39.4 Wed 10:30 H 1058

**Artificial tissue, Ultra-soft elastomers for cell mechanical investigation** — •Viktor Heinrichs[1,2], Sabine Dieluweit[1], Jörg Stellbrink[2], Rudolf Merkel[1], and Dieter Richter[2] — [1]ICS-7 Forschungszentrum Jülich GmbH, Jülich, Germany — [2]ICS-1 Forschungszentrum Jülich GmbH, Jülich, Germany

Most animal cells are strongly influenced by the elasticity and topography of their environment. For clear-cut investigation of cellular mechanobiology elastic model substrates are required. These materials should be biocompatible, transparent, suitable for micro structure fabrication and their elasticity should be tuneable in a wide range. However, a Young's modulus of 1 kPa (ultra-soft, necessary to model, e.g., brain or glial tissues) is difficult to achieve [1, 2]. These challenges can be tackled with cross-linked polydimethylsiloxane (PDMS) with the additional benefit of long shelf-life. We created a new PDMS material that meets all requirements in cell mechanics and examined it explicitly on viscoelastic properties with a strain controlled rheometer. The elasticity of the PDMS network was tuned via selection of the precursor polymers and their mixing ratio. Values as low as 1.5 kPa have been reliably achieved. First cell mechanical experiments on this novel material basis are underway. [1] C. M. Cesa, N. Kirchgeßner, D. Mayer, U. S. Schwarz, B. Hoffmann, R. Merkel. Rev. Sci. Instrum. 2007, 78, 034301. [2] D. T. Butcher, T. Alliston, V. M. Weaver, Nature Rev. Cancer 2009, 9, 108-122.

CPP 39.5 Wed 10:45 H 1058

**Molecular stress sensors constructed from DNA** — •Meenakshi Prabhune[1], Jonathan Bath[2], Andrew Turberfield[2], Florian Rehfeldt[1], and Christoph F Schmidt[1] — [1]Third Institute of Physics-Biophysics, Georg August University, Göttingen, Germany — [2]University of Oxford, Department of Physics, Clarendon Laboratory, Parks Road, Oxford OX1 3PU, UK

Molecular stress generation in cells is spatially and temporarily organized in complex patterns to drive meso-scale active processes such as intracellular transport, cell migration, or cell division. To quantitatively understand how these processes are driven, it is necessary to map local stresses inside cells, which is hard due to the lack of appropriate probes. We have designed a molecular-scale probe consisting of a self-assembled DNA hairpin with a fluorophore - quencher pair that responds to small forces applied to its ends. We demonstrate the working of this force sensor in vitro and explore possibilities for in vivo application to map local stress fields in cells.

CPP 39.6 Wed 11:00 H 1058

**Shape and adhesion dynamics of amoeboid cells studied by cell-substrate impedance fluctuations** — •Helmar Leonhardt — Universität Potsdam, 14476 Potsdam OT Golm

We present electrical impedance measurements of single amoeboid cells on microelectrodes. Wild type cells and mutant strains are studied that differ in their cell- substrate adhesion strength. We recorded the projected cell area by time lapse microscopy and found a correlation between kinetics of the projected area (cell shape oscillation) and the impedance long-term trend. We developed a data processing routine to extract such trends. We furthermore observed that cell-substrate attachment strength strongly affects the impedance in that the magnitude of fluctuations are enhanced in cells that effectively transmit forces to the substrate. For example, in talA- cells, which lack the actin anchoring protein talin, the fluctuations are strongly reduced. Such short-term fluctuations are extracted by high-pass filtering the original data. Typically, amoeboid motility advances via a cycle of membrane protrusion, substrate adhesion, traction of the cell body and tail retraction. This motility cycle results in the quasi-periodic oscillations of the projected cell area and the impedance. In all cell lines measured, similar periods were observed for this cycle, despite the differences in attachment strength. Based on the approach presented here, we can separate the changes in the impedance signal that are caused by the projected cell area from the fluctuations induced by the cell-substrate adhesion.

**30 min break**

CPP 39.7 Wed 11:45 H 1058

**Probing the role of cytoplasmic flows in embryogenesis** — •Matthäus Mittasch[1], Peter Gross[1,2], Stephan Grill[1,2], and Moritz Kreysing[1] — [1]Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden, Germany — [2]Biotechnology Center, Technische Universität Dresden, 01307 Dresden, Germany

While the genetic basis of embryogenesis is increasingly well understood, it is also clear that gene expression needs to be coupled to physical transport phenomena to account for the genesis of spatial structure. A striking example of morphogenesis is the polarization of the egg cell of the nematode worm C. elegans prior to asymmetric cell division. This process relies on the active cortical transport of morphogens (PAR proteins), and is impaired upon myosin-2 motor downregulation. However, little is known about the mechanistic role of the cytoplasmic flows that seem to stabilize cell polarization. Here, we adapt the previously described technique of light driven micro-fluidics (Weinert & Braun, J. appl. Phys. 2008), in order to now generate flows inside early stage embryos. Specifically, we report on the generation of micron-scale flow patterns confined in three dimensions, with velocities exceeding the wild type flows. By this, we aim to (i) rescue impaired embryos, (ii) manipulate wild-type cytoplasmic flow velocities, and (iii) introduce polarity multipoles through the induction of well-controlled artificial cytoplasmic flows inside C. elegans eggs. We anticipate that our findings will add to the general understanding of how biological systems utilize active transport phenomena to establish spatial structure.

CPP 39.8 Wed 12:00 H 1058

**Force fluctuations in three-dimensional suspended fibroblasts** — •Florian Schlosser, Christoph F. Schmidt, and Florian Rehfeldt — Drittes Physikalisches Institut - Biophysik, Georg-August-Universität Göttingen

Cells are sensitive to mechanical cues from their environment and at the same time generate and transmit forces to probe and to adapt to their surroundings. Key players in the generation of contractile forces are acto-myosin structures. To test forces and elasticity of cells not attached to a substrate, we used a dual optical trap to suspend 3T3 fibroblasts between two fibronectin-coated beads. We analyzed the correlated motions of the beads with high bandwidth. A combination of active and passive microrheology allowed us to measure the non-equilibrium force fluctuations as well as the elastic properties of the cell. We found that cortical forces deform the cell from its round shape in the frequency regime from 0.1 to 10 Hz. Biochemical perturbation experiments using blebbistatin for myosin inhibition and nocodazole for microtubule depolymerization show that cell stiffness and cortical force fluctuations highly depend on acto-myosin activity but not on microtubules. Serum-starvation also largely reduced the fluctuation amplitude. A force-clamp allowed us to observe cells under defined constant forces. Combining our optical trap with a confocal microscope allowed us to image the three-dimensional actin distribution of Life-Act transfected cells during the force measurements.

Schlosser, Rehfeldt, Schmidt, *Phil. Trans. R. Soc. B* 20140028, **2014**

CPP 39.9 Wed 12:15 H 1058

**Buckling dynamics of freely diffusing single erythrocytes** — •Michael Göllner, Adriana C. Toma, and Thomas Pfohl — Department of Chemistry, University of Basel, Switzerland

Containing a wealth of information, human blood is the most used sample for diagnostic purposes. Microfluidics, with its unique advantages in performing analytical functions, has been increasingly used for whole blood and cell-based analysis. However, studies on the single-cell level using microfluidic techniques often require active immobilization in order to be investigated by optical methods.

We developed a microfluidic setup for single red blood cell (RBC) assays starting with whole blood samples which permits diffusion-controlled variation of the external environment. Individual RBCs are freely diffusing inside microchambers without adhesive interactions to the glass coverslip or the use of optical tweezers. By increasing the surrounding osmotic pressure, erythrocytes are exhibiting a buckling transition which is described by means of radial Fourier analysis. Temporal evolution of the modal decomposition of cell edge movement leads to characterization of osmolarity-dependent fluctuations of freely diffusing single RBCs.

CPP 39.10 Wed 12:30 H 1058

**Biomechanics of the Spinal Cord** — •David E. Koser and Kristian Franze — Department of Physiology, Development and Neuroscience, University of Cambridge, United Kingdom.

In cell physiology and pathology mechanical signaling plays an important role. Many cell types, including central nervous system cells, respond to the mechanical cues in their environment. Yet, in spinal cord, data on tissue stiffness are sparse and therefore the mechanical environment is unknown. To fill this gap, we conducted atomic force microscopy indentation and tensile measurements on acutely isolated mouse spinal cord tissue sectioned along the three major anatomical planes (transverse, coronal and sagittal planes), and correlated local mechanical properties with the underlying cellular structures. Our measurements revealed that gray matter is significantly stiffer than white matter irrespective of directionality and force direction. While white matter behaved like a transverse isotropic material on all length scales, gray matter was isotropic at the tissue and anisotropic at the cellular scale. Most importantly, tissue stiffness correlated with axon orientation, cell body size, and cellular in plane proximity, which we combined into a linear model to estimate local central nervous system tissue stiffness. Our study may thus lay the foundation to predicting local tissue stiffness based on histological data, and hence contribute to the understanding of cell behavior in response to mechanical signaling under physiological and pathological conditions.

CPP 39.11 Wed 12:45 H 1058

**Properties of Single Squamous Cell Carcinoma Cells** — •Susanne Steeger[1], Tanja Schreyer[1], Stefan Hansen[2], Jörg Schipper[2], and Mathias Getzlaff[1] — [1]Heinrich-Heine-Universität Düsseldorf, Deutschland — [2]Univ.-HNO-Klinik Düsseldorf, Deutschland

In this contribution we report on measurements of the mechanoelastic properties of ENT squamous cell carcinoma cells. The study of these single cancer cells in culture medium is carried out by Atomic Force Microscopy. Our main interest is the determination oft the Youngs Modulus calculated by the Hertzian Model. We identify the elasticity of cancer cells in order to compare it with that of similar benign cells. Because Live Cell Imaging is a challenging task we first focus on testing different cantilevers and various strategies to treat the cells carefully. In order to determine the individual properties of the cancer cells we additionally analyse their cytoskeleton (actin and tubulin) by using a confocal fluorescence microscope. Cancer cells are known for their modified cytosekelton which is reflected in the different elasticities of both cancer and comparable benign cells.

CPP 39.12 Wed 13:00 H 1058

**PAR polarity pattern in C. elegans zygotes establishes via**

**a mechanochemical feedback module** — •Peter Gross[1,2], K.Vijay Kumar[2,3], Nathan W. Goehring[4], Justin S. Bois[5], Frank Jülicher[3], and Stephan W. Grill[1,2,3] — [1]MPI-CBG, Dresden — [2]BIOTEC, TU Dresden — [3]MPI-PKS, Dresden — [4]London Research Institute, UK — [5]UCLA, Los Angeles, CA

The interplay between biochemistry and cell mechanics is critical for a broad range of morphogenetic changes. A prominent example hereof is the emergence of cell polarity during the embryogenesis of C. elegans, resulting in a patterned state of the membrane-associated PAR polarity proteins. Crucial for the emergence of the patterned state are large-scale flows in the membrane-associated actomyosin cortex, which are observed concomitantly with the emergence of PAR polarization. The coupling of biochemistry and cortical flows, driving this mechanochemical patterning processes, remain poorly understood. Here we establish that PAR polarization of C. elegans zygotes represents a coupled mechanochemical feedback system. We demonstrate that the biochemistry in form of the PAR domains controls mechanics by establishing a myosin gradient. We measure the spatiotemporal profile of the anterior and posterior PAR concentration, the myosin concentration and the induced flow-field. Furthermore we present a theoretical description of this process in the framework of active fluids combined with PAR biochemistry in a coupled reaction-diffusion active-fluids approach. We show that this mechanochemical feedback description quantitatively recapitulates the spatiotemporal profile of PAR polarity emergence.

# CPP 40: Charged Soft Matter II

Time: Wednesday 9:30–11:30 Location: PC 203

CPP 40.1 Wed 9:30 PC 203

**Molecular Dynamics Simulations of Ultracentrifuged Polyelectrolyte Complexes** — •Diddo Diddens, Albert Johner, and Jörg Baschnagel — Institut Charles Sadron, Université de Strasbourg, 23 Rue du Loess, BP 84047, 67034 Strasbourg Cedex 2

Polyelectrolyte complexes (PECs) are formed by the aggregation of positively and negatively charged polymer species, which precipitate rapidly from solution in case of equimolar mixing. As the fast complexation kinetics prevents the formation of an optimized pairing between positive and negative charges, the microstructure of these aggregates is ill-defined, resulting in a material that is difficult to process further.

Recently, Schlenoff *et al.* [1] have demonstrated that the precipitates can be reshaped via ultracentrifugation in concentrated sodium chloride solutions, yielding a compacted, gel-like material, whose rheological properties make them interesting candidates for bioimplants [2]. However, despite the success of this novel route to post-process PECs, the underlying molecular mechanisms are not yet fully resolved.

We study the complex structure before, during and after centrifugation in a non-equilibrium Molecular Dynamics simulation of a fully atomistic simulation model. In a second step, we investigate the effect of these structural changes on the dynamics inside the PECs, and discuss these findings in context with the experimental observations.

[1] Porcel and Schlenoff, *Biomacromolecules*, **2009**, 10, 2968

[2] Hariri and Schlenoff, *Macromolecules*, **2010**, 43, 8656

CPP 40.2 Wed 9:45 PC 203

**Coarse-grained models for simulations of polyelectrolyte multilayers and complexes** — •Martin Vögele[1,2], Jens Smiatek[1], and Christian Holm[1] — [1]Institut für Computerphysik, Universität Stuttgart — [2]Max-Planck-Institut für Biophysik, Frankfurt am Main

We present coarse-grained models for the polyelectrolytes Poly(styrene sulfonate) (PSS) and Poly(diallyldimethylammonium) (PDADMA) in terms of a MARTINI based approach. Our models allow us to study the properties of polyelectrolyte complexes and polyelectrolyte multilayers on large length and long time scales while still taking into account chemical details. In our simulations, we use the new polarizable coarse-grained MARTINI water model. We further studied the behavior of this water model in presence of varying sodium chloride concentrations. The numerical findings are compared to experimental results and atomistic models.

Our results validate that the MARTINI water model can be used to reproduce the properties of aqueous salt solutions in good agreement to atomistic models. The polyelectrolyte models further reproduce the correct charge compensation mechanism as well as the recently observed lower water dielectric constants which can both be interpreted as the underlying reasons for the stability of polyelectrolyte multilayers and complexes.

CPP 40.3 Wed 10:00 PC 203

**Absorption of a polyelectrolyte star by an oppositely charged polyelectrolyte brush: A molecular dynamics simulation study** — •Majid Farzin[1,2], Torsten Kreer[1], and Jens-Uwe Sommer[1,2] — [1]Leibniz Institute for Polymer Research Dresden — [2]Technische Universitaet Dresden

By means of molecular dynamics simulations, we study interactions between a polyelectrolyte brush and an oppositely charged polyelectrolyte star. We explicitly include counter-ions of two different sizes and vary the strength of Coulomb interactions in two ways; by varying the Bjerrum length of fully charged polyelectrolytes and by choosing different charge fractions of polyelectrolyte brush monomers for a Bjerrum length corresponding to the value in water. Simulations show that there is a Bjerrum length at $10^{-3}$ (Lennard-Jones units) above which the polyelectrolyte star undergoes a discontinuous absorption transition by the polyelectrolyte brush. For a Bjerrum length of $10^{-2}$ the polyelectrolyte star has the minimum extension in the direction perpendicular to the brush. Finally, for a Bjerrum length of 0.5 the polyelectrolyte brush undergoes a collapse transition.

CPP 40.4 Wed 10:15 PC 203

**Stimuli-responsive polyampholyte hydrogels - influence of charge asymmetry and ionic strength** — •Margarita Dyakonova[1], Maria T. Popescu[2], Konstantinos Kyriakos[1], Sebastian Jaksch[3], Constantinos Tsitsilianis[2], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Physik weicher Materie, Garching — [2]University of Patras, Greece — [3]JCNS at FRM II, Garching

We investigate the rheological and structural properties of physical hydrogels, formed via charge driven self-association of triblock polyampholytes PAA-P2VP-PAA and PAA-QP2VP-PAA (PAA, P2VP and QP2VP are poly(acrylic acid), poly(2-vinylpyridine) and quaternized poly(2-vinylpyridine)), which have attracted a considerable interest for use as injectable hydrogels and drug carriers. Both, the PAA and P2VP blocks are ionizable. PAA is deprotonated at high pH, whereas P2VP is positively charged at low pH. QP2VP is highly charged, independently of pH. In water, the gelation threshold is at 1.0 wt% [1]. Small-angle neutron scattering (SANS) experiments revealed the morphological changes depending on the charge asymmetry. The structure develops from uncorrelated globular aggregates to a network. These findings corroborate the ones from rheological studies, implying the formation of stiff hydrogels at low pH. Ionic strength is an alternative way of controlling the strength of electrostatic interactions. Combined SANS and rheological studies have revealed a different structure revolution inside the polyampholyte networks depending on ionic strength. [1] N. Stavrouli et al., Polymer 49, 1249 (2008).

CPP 40.5 Wed 10:30 PC 203

**Specific salt effects on thermophoresis of charged colloids** — •Arghya Majee[1], Kyriakos A. Eslahian[2], Michael Maskos[2], and Alois Würger[3] — [1]Max Planck Institute IS & University of Stuttgart, Germany — [2]Fraunhofer ICT-IMM, Mainz, Germany — [3]LOMA, Université de Bordeaux & CNRS, France

The electrolyte Seebeck effect determines to a large extent the properties of charged colloids that are heated or subject to a thermal gradient. The electric double layer responds to a non uniform temperature through several mechanims, resulting in a significant thermocharge and transport to the hot or to the cold side [1]. In this contribution we discuss the Soret effect of charged polystyrene particles as a function of temperature and electrolyte composition [2]. As a main result we find that the Soret coefficient is determined by charge effects, and that nonionic contributions are small. In view of the well-known electric-double layer interactions, our thermal field-flow fractionation data lead us to the conclusion that the Soret effect originates to a large extent from diffusiophoresis in the salt gradient and from the electrolyte Seebeck effect, both of which show strong specific-ion effects. Moreover, we find that thermophoresis of polystyrene beads is fundamentally different from proteins and aqueous polymer solutions, which show a strong non-ionic contribution.

References:

[1] A. Majee, A. Würger, Phys. Rev. Lett. **108**, 118301 (2012).

[2] Kyriakos A. Eslahian, A. Majee, M. Maskos, and A. Würger, Soft Matter **10**, 1931 (2014).

CPP 40.6 Wed 10:45 PC 203

**Molecular dynamics simulation of sulfone linked sulfonated dimers** — •anand narayanan krishnamoorthy[1], jens smiatek[2], and christian holm[3] — [1]Institute for Computational Physics,University of Stuttgart — [2]Institute for Computational Physics,University of Stuttgart — [3]Institute for Computational Physics,University of Stuttgart

This project focuses on the investigation of structural properties of sulfone linked sulfonated dimers in lithium form via all atom molecular dynamics simulations. Previous research has been primarily focused on sulfonated polyelectroytes in apolar and aprotic solvents in sodium form. But it is quite interesting to study the conformations and binding mechanisms of these typical dimers in lithium form in a braod range of solvents. The results show that the typical conformations of these dimers plays a vital role in determining the suitable ion binding mechanism to the dimer. Triple binding mechanism is favored for sulfonic acid ortho form of the dimer where a single and double binding mechanism is favored for the meso form. Also the condensation behavior of these dimers were studied under various aprotic, protic, polar and apolar solvents.

CPP 40.7 Wed 11:00 PC 203

**Mechanisms underlying reentrant phase behavior of proteins: a model system** — •Michal Braun[1], Marcell Wolf[1], Olga Matsarskaia[1], Gudrun Lotze[2], Fajun Zhang[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]ESRF, Grenoble, France

Controlling and tuning the phase behavior of proteins is important in many areas such as structural biology including protein crystallization, pharmacology and biotechnology. One important effect in protein phase behavior is reentrant condensation (RC) which can be induced and controlled by multivalent ions ([1], [2], [3]). For example, $YCl_3$ leads to RC in bovine serum albumin (BSA). This system features a macroscopic phase separation, which makes it difficult to study the mechanisms behind RC using scattering. $LaCl_3$, on the other hand, induces cluster formation and RC in BSA without phase separation and the BSA-$LaCl_3$ system is therefore highly suitable for the study of the physical mechanisms behind RC. Here, we discuss our findings from systematic SAXS and light scattering (LS) experiments as a function of both protein and salt concentrations. SAXS curves can be fitted using a sticky hard sphere model and the reentrant behavior is reflected in the stickiness parameter. LS helps to reveal the dependency of the cluster sizes on the interactions. These measurements thus provide detailed insights into the interactions in a system featuring RC. [1] Zhang et al., *PRL*, **101**, 148101, 2008, [2] Zhang et al., *Soft Matter*, **8**, 1313, 2012, [3] Roosen-Runge et al., *PNAS*, **108**, 11815, 2011

CPP 40.8 Wed 11:15 PC 203

**The effect of variable charge patterns: interactions and phase behaviour of a non-monoclonal antibody mixture** — •Stefano Da Vela[1], Fajun Zhang[1], Michael Sztucki[2], Ralf Schweins[3], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]ESRF, Grenoble, France — [3]ILL, Grenoble, France

Bovine $\gamma$-globulin is an easily available mixture of antibodies (immunoglobulins) with different specificities: this implies that the constituents feature a manifold of surface charge distribution patterns. The main component is Immunoglobulin G (IgG), an anisotropic, Y-shaped protein. We aim to understand the relationship between the profusion of anisotropic charge driven interactions present in the system and the macroscopic phase behaviour. Solutions of $\gamma$-globulin in a wide range of protein volume fractions (0.001 up to 0.27) are investigated with and without added salts using predominantly turbidimetry, dynamic light scattering, small angle x-ray and neutron scattering. We show how the heterogeneity of the charge distribution in different proteins accounts for sample bidispersity and explains self-association and turbidity in $\gamma$-globulin dispersions at low ionic strengths. At high volume fractions, the repulsive component of the effective interaction is modelled considering protein anisotropy. Our work has potential applications in the stability enhancement of analogous therapeutic blood products.

## CPP 41: Optical and Nonlinear Optical Properties I (joint session DF, CPP)

Time: Wednesday 9:30–11:00 Location: EB 407

**Invited Talk** CPP 41.1 Wed 9:30 EB 407

**Holographic microstructuring of liquid-crystalline elastomers** — •Irena Drevensek-Olenik[1,2], Martin Čopič[1,2], Martin Fally[3], Valentina Domenici[4], and Antoni Sánchez-Ferrer[5] — [1]Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19, SI1000 Ljubljana, Slovenia — [2]J. Stefan Institute, Jamova 39, SI1000 Ljubljana, Slovenia — [3]Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Wien, Austria — [4]Dipartimento di Chimica e Chimica Industriale, Università degli studi di Pisa, via Risorgimento, 35, 56126 Pisa, Italy — [5]Department of Health Sciences and Technology, ETH Zurich, Schmelzbergstrasse 9, 8091 Zurich, Switzerland

Adding a small amount of photoactive component, for instance a photo-isomerizable azobenzene derivative, to the matrix of a liquid-crystalline elastomer (LCE) opens up various possibilities for optical manipulation of mechanical, thermal, electrical and optical properties of the material. Holographic microstructuring in LCEs is based on the coupling between isomerization state of the azobenzene groups and orientational order of the mesogenic side chains. Due to collective nature of this process light-induced spatial modifications of optical refractive index in LCEs are several magnitudes larger than in conventional azobenzene-based holographic media. Holographic patterning of LCEs consequently provides a very convenient method for fabrication of tuneable optical diffraction structures that can easily be manipulated by external stimuli, such as strain, external fields and temperature variations.

CPP 41.2 Wed 10:00 EB 407

**Random-Cavity Lasing from Electrospun Polymer Fiber Networks** — •Sarah Krämmer[1], Christoph Vannahme[2], Cameron L. C. Smith[2], Tobias Grossmann[1], Michael Jenne[1], Stefan Schierle[1], Minh Tran[1], Lars Jørgensen[3], Ioannis S. Chronakis[3], Anders Kristensen[2], and Heinz Kalt[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), Germany — [2]Department of Micro- and Nanotechnology, Technical University of Denmark (DTU), Denmark — [3]DTU-Food, DTU, Denmark

Electrospinning is a versatile, simple, low-cost and high-throughput technique for the fabrication of fibers and fiber networks with fiber diameters in the micro- and nanometer range. The resulting high surface-to-volume ratio makes the fibers excellent candidates for sensing, tissue-growth and filtering. In the field of photonics they serve as waveguides and light sources when doped with an emitter. We report on the lasing emission from random cavities formed in networks of electrospun dye-doped polymer fibers. Spatially resolved spectroscopy and spectral analysis prove that the observed laser emission originates from individual ring resonators randomly distributed throughout the network. Preliminary measurements show the suitablity of the fiber networks as gas sensors where the spectral position of a lasing mode serves as transducer.

CPP 41.3 Wed 10:20 EB 407

**Whispering Gallery Modes in Single Copolymer Microspheres** — •Daniel Braam[1], Kenichi Tabata[2], Soh Kushida[2], Robert Niemöller[1], Günther M. Prinz[1], Yohei Yamamoto[2], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany — [2]Faculty of Pure and Applied Sciences, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8573, Japan

Copolymers are promising candidates for use in optoelectronic devices due to their low fabrication cost and high emission efficiency. Here we investigate several $\pi$-conjugated alternating copolymers, which combine the advantages of being a dye, a dielectric and a self-assembled resonator, as they form nearly perfect spheres when precipitated from solution. Excitation leads to standing waves inside these microspheres, known as whispering gallery modes (WGMs). Their spectral position, number and line width is dependent on the sphere diameter. The measurements, showing both TM- and TE-modes, are in good agreement with model calculations [1]. The relative amplitude of the modes is strongly dependent on the sphere's excitation spot, revealing leakage of polar modes to the substrate, while equatorial modes sustain. During continuous illumination we observe lifting of degeneracy of the WGMs, followed by slow deterioration. Covering the spheres with a thin layer of titanium leads to an improved resistance against irradiation damage.

[1] Tabata, K., Braam, D. *et al.* Self-assembled conjugated polymer spheres as fluorescent microresonators. Sci. Rep. **4**, 5902; DOI:10.1038/srep05902 (2014).

CPP 41.4 Wed 10:40 EB 407

**$TiO_2$ coated Whispering Gallery Mode (WGM) Resonators for Label-free Biosensing** — •Fabian Ruf[1], Sarah Krämmer[1], Christoph Vannahme[2], Antonina Vigovskaya[3], Ljiljana Fruk[3], Anders Kristensen[2], and Heinz Kalt[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), Germany — [2]Department of Micro- and Nanotechnology, Technical University of Denmark (DTU), Denmark — [3]DFG-Centre for Functional Nanostructures CFN, Karlsruhe Institute of Technology (KIT), Germany

Biosensors for label-free detection offer a huge variety of applications in life sciences and medicine since they facilitate point-of-care diagnostics. We use goblet-shaped polymeric high-Q WGM microresonators fabricated within a low-cost manufacturing process also suitable for mass production. After fabrication the polymeric resonators are coated with titanium dioxide using sputter deposition techniques. The sensitivity as figure of merit is given here by the size of the shift of a resonant mode when the surrounding of the resonator changes. Finite element simulations predict a significantly increased sensitivity for resonators coated with $TiO_2$. Moreover, titanium dioxide is a well-suited platform for functionalization with dopamine derivates. The use of antibody-protein binding processes is expected to enable the specific detection of proteins and antibodies interesting for medical analysis.

## CPP 42: Transport: Fluctuations and Noise (joint session TT, CPP, DY)

Time: Wednesday 11:30–12:45 Location: H 3005

CPP 42.1 Wed 11:30 H 3005

**Quantum transport, master equations, and exchange fluctuations** — •Sigmund Kohler and Robert Hussein — Instituto de Ciencia de Materiales de Madrid, CSIC, 28049 Madrid, Spain

We investigate to which extent a many-body Bloch-Redfield master equation description of transport in coupled quantum dots is consistent with the exact generalized equilibrium conditions known as exchange fluctuation theorems. Thereby we identify a class of master equations for which this is the case. Beyond this class, we find deviations which exhibit characteristic scaling laws as functions of the dot-lead tunneling, the inter-dot tunneling, and the temperature. These deviations are accompanied by an increase of lead energy fluctuations inherent in the Bloch-Redfield equation beyond rotating-wave approximation. We illustrate our results with numerical data for a double and a quadruple quantum dot attached to four leads.

[1] R. Hussein and S. Kohler, Phys. Rev. B **89**, 205424 (2014).

CPP 42.2 Wed 11:45 H 3005

**Waiting time-distribution of a quantum-dot spin valve** — •Björn Sothmann — Département de Physique Théorique, Université de Genève, Genève, Switzerland

Recently, the study of waiting-time distributions of electron transport has received a lot of interest [1]. It can provide information about transport processes that is complementary to average current and noise. Here, we discuss the waiting-time distribution of a a quantum-dot spin valve [2], i.e., a single-level quantum dot coupled to two ferromagnetic electrodes with magnetizations that can point in arbitrary directions [3]. We demonstrate that the rich transport physics of this setup, such as the dynamical channel blockade and spin precession in an interaction-driven exchange field, shows up in the waiting-time distribution, and we analyze the conditions necessary to observe the various effects.

[1] M. Albert, G. Haack, C. Flindt, M. Büttiker,
Phys. Rev. Lett. **108**, 186806 (2012).
[2] B. Sothmann, Phys. Rev. B **90**, 155315 (2014).
[3] M. Braun, J. König, J. Martinek,
Phys. Rev. B **70**, 195345 (2004).

CPP 42.3 Wed 12:00 H 3005

**Waiting-time distribution of light from superconducting resonators coupled to voltage-biased Josephson junctions** — •Simon Dambach, Björn Kubala, Vera Gramich, and Joachim Ankerhold — Institute for Complex Quantum Systems, Ulm University, Ulm, Germany

The interplay of the tunneling transfer of charges and the emission and absorption of light can be investigated in a set-up, where a voltage-biased Josephson junction is placed in series to a microwave cavity. In such devices measurements of the emitted microwave radiation can yield information about the Cooper pair current and its fluctuations and vice versa.

Due to the inherent nonlinearity of the Josephson junction tunneling Cooper-pairs can create a variety of non-classical states of light already at weak driving. Depending on experimental parameters and tuning, the device can be described by effective Hamiltonians, indicating specific photon creation mechanisms which lead to strongly bunched or anti-bunched light emission [1].

We will use the waiting-time distribution [2] of emitted photons to highlight how charge quantization of the Cooper pair current drives a crossover from a coherent light source to a single-photon source. Analytical results for the weak driving regime, based on a quantum regression approach, are complemented by numerical results for the full nonlinear quantum case.

[1] B. Kubala, V. Gramich, and J. Ankerhold, arXiv:1404.6259.
[2] T. Brandes, Ann. Phys. (Berlin) **17**, 477 (2008).

CPP 42.4 Wed 12:15 H 3005

**Input-output description of microwave radiation in the dynamical Coulomb blockade** — Juha Leppäkangas[1], Göran Johansson[1], •Michael Marthaler[2], and Mikael Fogelström[1] — [1]Microtechnology and Nanoscience, MC2, Chalmers Universit y of Technology, SE-412 96 Göteborg, Sweden — [2]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany

We study microwave radiation emitted by a small voltage-biased Josephson junction connected to a superconducting transmission line. An input-output formalism for the radiation field is established, using a perturbation expansion in the junction's critical current. Using output field operators solved up to the second order, we estimate the spectral density and the second-order coherence of the emitted field. For typical transmission line impedances and at frequencies below the main emission peak at the Josephson frequency, radiation occurs predominantly due to two-photon emission. This emission is characterized by a high degree of photon bunching if detected symmetrically around half of the Josephson frequency. Strong phase fluctuations in the transmission line make related nonclassical phase-dependent amplitude correlations short lived, and there is no steady-state two-mode squeezing. However, the radiation is shown to violate the classical Cauchy-Schwarz inequality of intensity cross-correlations, demonstrating the nonclassicality of the photon pair production in this region.

CPP 42.5 Wed 12:30 H 3005

**Distribution of energy dissipated by a driven two-level system** — •Philip Wollfarth[1,2], Alexander Shnirman[1,2], and Yasuhiro Utsumi[3] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]DFG Center for Functional Nanostructures (CFN), Karlsruhe Institute of

Technology, 76128 Karlsruhe, Germany — [3]Department of Physics Engineering, Faculty of Engineering, Mie University, Tsu, Mie, 514-8507, Japan

In the context of fluctuation relations, we study the distribution of energy dissipated by a driven two-level system. Incorporating an energy counting field into the well known spin-boson model enables us to calculate the distribution function of the amount of energy exchanged between the system and the bath. We also derive the conditional distribution functions of the energy exchanged with the bath for particular initial and/or final states of the two-level system. We confirm the symmetry of the conditional distribution function expected from the theory of fluctuation relations. We also find that the conditional distribution functions acquire considerable quantum corrections at times shorter or of the order of the dephasing time. Our findings can be tested using solid-state qubits.

[1] P. Wollfarth, A. Shnirman, Y. Utsumi,
Phys. Rev. B **90**, 165411 (2014).

## CPP 43: P8: Nanoparticles and Compsite Materials

Time: Wednesday 10:00–13:00 Location: Poster A

CPP 43.1 Wed 10:00 Poster A

**The Effect of preparation method on the physical properties and the dynamic glass transition of the nanocomposites based on hyperbranched polymers** — •Shereen Omara[1], Mona Abdel Rehim[2], Ahemd Ghoneim[3], Sherif Madkour[1], Gamal Turky[3], and Andreas Schönhals[1] — [1]Federal Institute for Materials Research and Testing (BAM), Unter den Eichen 87, D-12200 Berlin, Germany — [2]Packing and Packaging Materials Department, National Research Center, Cairo, Egypt — [3]Microwave Physics and Dielectrics Department,National Research Center, Cairo, Egypt

Broadband dielectric spectroscopy, Specific heat spectroscopy, and Differential scanning calorimetry (DSC) are combined to study the glass transition and segmental motions in hyperbranched polyamine ester (HB PAE) and its nanocomposite with kaolinite (Ka). In situ polymerization and solution mixing (Ex situ) are applied to prepared HB-PAE/Ka nanocomposites with different concentrations of Ka.The dielectric spectra are dominated on the lower frequency (higher temperature) side by conductivity contribution. The molecular dynamic is found to be screened out by the conductivity contribution; otherwise Specific heat spectroscopy was used to determine the dynamic glass transition temperature of HBPs/Ka nanocomposite. The segmental motion related to the glass transition called alpha process found to play a role in the charge transport. The result indicated that the dc conductivity and the dynamic glass transition temperature depend not only on different concentrations of kaolinite but also on the method of the preparation of the nanocomposite.

CPP 43.2 Wed 10:00 Poster A

**Positioning of magnetic particles in polymer matrices for smart material engineering by magnetically patterned exchange bias templates** — •Iris Koch[1], Markus Langner[2], Andreas Greiner[2], and Arno Ehresmann[1] — [1]Department of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel — [2]Department of Macromolecular Chemistry II, University of Bayreuth, Universitätsstr. 30, D-95440 Bayreuth

Magnetic micro-stripe patterned exchange bias systems with different stripe widths were used as a template for the precise positioning of either pure ferromagnetic nanoparticles or superparamagnetic core-shell microspheres in polymer thin film systems. The positioning was assisted by an out-of-plane magnetic field superimposing the magnetic field landscape of the exchange bias substrate. The particle/polymer composite was subsequently obtained via lift-off from the magnetically patterned template. An interaction with external magnetic fields was observed in air and in liquid environment down to a mass fraction of 3 % magnetic material in relation to the polymeric material.

CPP 43.3 Wed 10:00 Poster A

**Thermoelectric thin films based on a polymer/nanoparticle nanocomposite** — •Nitin Saxena[1,2], Anton Greppmair[3], Mihael Coric[4], Jan Wernecke[5], Stefanie Marggraf[5], Eva M. Herzig[4], Martin S. Brandt[3], and Peter Müller-Buschbaum[1,2] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Center for NanoScience, LMU München, 80539 München, Germany — [3]TU München, Walter-Schottky-Institut and Physik-Department, 85748 Garching, Germany — [4]TU München, Munich School of Engineering, 85748 Garching, Germany — [5]Physikalisch-Technische Bundesanstalt, BESSY II Helmholtz-Zentrum Berlin, 12489 Berlin, Germany

Thermoelectric materials transform temperature gradients into voltages which can be used to generate electrical power. Highly efficient thermoelectrics comprise rare and/or toxic inorganic materials and require cost- and energy-intensive fabrication processes. This impedes their large-scale application for power generation.

In order to overcome these limitations, we pursue a hybrid approach combining the semiconducting polymer blend PEDOT:PSS for its high electrical conductivity and inorganic nanoparticles in order to reduce thermal conductivity within the thin film. We investigate the influence of the nanoparticles on the morphology of the blend by means of GISAXS and attempt to correlate this with changes in the thermoelectric behavior. Apart from that, we also investigate the thermal conductivity of both pristine PEDOT:PSS and of the hybrid film, in order to ultimately calculate the figure-of-merit ZT.

CPP 43.4 Wed 10:00 Poster A

**Structural study of magnetic nanoparticle-block copolymer hybrid films prepared by printing techniques** — •Senlin Xia, Yuan Yao, Ezzeldin Metwalli, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Metal-polymer nano-composites are an important class of hybrid materials due to their interesting functional applications, e.g. sensors, and memory devices [1,2]. Hybrid films of magnetite nanoparticles and the diblock copolymer (DBC) poly(styrene-b-methyl methacrylate) are prepared using a printing method, with the potential of high mass production and energy saving. The relationship between viscosity of nanoparticle-polymer solution and the film formation was carefully explored in order to find the optimized processing conditions. The printed hybrid films are investigated using both real-space and reciprocal-space techniques. The nano- and microstructure of maghemite nanoparticles within DBC films as a function of the nanoparticle concentration is investigated using optical microscopy, atomic force microscopy, scanning electron microscopy and grazing incidence small-angle X-ray scattering. The magnetic property of the hybrid films is probed using a superconducting quantum interference device (SQUID) magnetometer. The observed structures are explained in the framework of microphase separation and confinements. A comparison of the nano-morphology between the spin-coated and printed hybrid films is discussed. [1] Y. Yao, et.al. ACS Appl. Mater. Interfaces 6, 5244, (2014); [2] Y. Yao et.al. ACS Appl. Mater. Interfaces 6, 18152, (2014).

CPP 43.5 Wed 10:00 Poster A

**Structure-Property relationships of Nanocomposites Based on Polylactide and Layered Double Hydroxides** — •Jing Leng[1], De-Yi Wang[2], Andreas Thünemann[1], Franziska Emmerling[1], Andreas Wurm[3], Christoph Schick[3], and Andreas Schönhals[1] — [1]BAM Federal Institute for Material Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany — [2]IMDEA Materials Institute, C/Eric Kandel 2, 28906 Getafe, Madrid, Spain — [3]University of Rostock, Institute of Physics, Wismarsche Str. 43-45, 18051 Rostock, Germany

Two kinds of Polymer based nanocomposites prepared by melt blending of synthesized NiAl (NiAl-LDH) and MgAl (MgAl-LDH) layered double hydroxides with polylactide (PLA) 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). By detailed colorimetric investigations (stepscan DSC) the rigid amorphous phase due to the both the crystals and the nanoparticles was estimated unambiguously. A higher rigid amorphous fraction (RAF) due to the nanoparticles exists in the case of MgAl-LDH based nanocomposites compared to NiAl-LDH based nanocomposites. The dielectric spectra of the both nanocomposites showed several relaxation processes related to dynamic glass transition and localized fluctuations that were identified and analyzed in detail.

CPP 43.6 Wed 10:00 Poster A

**Structure-Property relationships of Nanocomposites Based on Epoxy and Layered Double Hydroxides** — •Jing Leng[1], Franziska Emmerling[1], De-Yi Wang[2], and Andreas Schönhals[1] — [1]BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany — [2]IMDEA Materials Institute, C/Eric Kandel 2, 28906 Getafe, Madrid, Spain

Two kinds of organically modified MgAl Layered Double Hydroxides (MgAl-LDH) were synthesized and reaction blended with an epoxy system (EP) to obtain polymer based nanocomposites. The organic modification of the MgAl-LDHs were by sodium dodecylbenzene sulfonate (SDBS) modified and own synthesized nanofiller (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 43.7 Wed 10:00 Poster A

**Morphology investigation of self-assembly of metal oxide-diblock copolymer nanocomposite films** — •Yuan Yao[1], Ezzeldin Metwalli[1], Jean-Francois Moulin[2], Matthias Opel[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]HZ Geesthacht at FRM II, Lichtenbergstr.1, 85748 Garching, Germany — [3]Walther-Meissner-Institut, Walther-Meissner-Str. 8, 85748 Garching, Germany

The arrangement of maghemite nanoparticles (NPs) in diblock copolymer poly (styrene-d8-block-n-butyl methacrylate) P(Sd-b-BMA) films via a self-assembly process is investigated. This study is motivated by great interests for many potential applications in functional nanodevices. The resulting hybrid thin films show a perforated lamella structure with an enrichment layer containing different NPs concentrations (from 0 up to 15 wt%) as investigated with X-ray reflectometry, scanning electron microscopy, atomic force microscopy, and grazing incidence small angle neutron scattering in time-of-flight mode (TOF-GISANS). The surface modified NPs are selectively positioned in one polymer domain at low NP concentrations and the microphase separation process is even enhanced in this case. However, a distortion of the lamella structure evolves with increasing NP concentrations.

CPP 43.8 Wed 10:00 Poster A

**Polymer metal oxide hybrid materials and films** — •Michael Bahr, Ezzeldin Metwalli, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Materials with novel electrical, optical and magnetic properties are possible thanks to the implementation of metal-polymer nanocomposite (MPN) structures. In future, thin films of MPN will be suitable for applications like sensors and memory devices. In such composites diblock copolymers are the matrix of choice for providing the desired arrangement of the metal, since they exhibit structure formation due to micro phase separation. Metal attaches preferentially to one of the two copolymer blocks, thereby forming a well-ordered structure inside the polymer matrix.

In this work we use an in-depth investigation of the system poly(strerene-b-methylmethacrylate) (PS-b-PMMA), which forms a lamellar structure, and a Cobalt salt based on a 2,2' bipyridine ring ($C_{10}H_8Cl_2CoN_2$). Bulk samples and thin films are prepared with different molar ratios of the salt and block copolymer by solution casting and by spin coating, where the cobalt content oxidizes. Bulk samples are characterized with in-situ thermal SAXS. Thin films are investigated with FTIR, AFM and SEM. We observe a well-ordered structure of the polymer matrix and a change of morphology with different molar ratios.

CPP 43.9 Wed 10:00 Poster A

**Gastransport Properties and Molecular Mobility of Matrimid/PhenethylPOSS Nanocomposites** — •Nora Konnertz, Martin Boehning, and Andreas Schoenhals — BAM Federal Institute of Materials Research and Testing, Unter den Eichen 87, 12205 Berlin

Polymers are favored materials for gas separation membranes. The development of new material with higher permeabilities and selectivities is challenging because the structure and property optimization follows a trade-off: improvements of permeability is often connected to a reduction in selectivity and vice versa. A promising approach for improvements is the incorporation of nanoscaled fillers. In order to understand thus induced changes in the solution-diffusion mechanism (which describes the gas transport through polymer membranes) in more detail it is important to relate the molecular mobility of the polymer in the nanocomposites with the gas transport properties. Here this relation is studied using Matrimid5218 as polymer matrix and a polyhedral oligomeric silsesquioxane with phenethyl substituents (Phenethyl-POSS) as nanofiller. Films with filler contents up to 20 wt% were casted from dichloromethane solution (thicknesses around 100 $\mu$m). The molecular mobility is determined by broadband dielectric spectroscopy. Permeabilities were measured with the time-lag method (0 - 20 bar) and sorption by using a microbalance (0 - 45 bar) for different gases.

CPP 43.10 Wed 10:00 Poster A

**QCM System for the Characterization of Gas Sorption and Physical Aging on Membrane Polymers and Nanocomposites for Gas Separation Applications** — •Nora Konnertz and Martin Boehning — BAM Federal Institute of Materials Research and Testing, Unter den Eichen 87, 12205 Berlin

The Quartz Crystal Microbalance (QCM) is a very sensitive method to detect mass changes in a range of nanograms. Thus this method enables sorption experiments with thin films or layers attached to the QCM crystal (in a range up to 1 $\mu$m). Here we present the experimental set-up for using the QCM technique for characterizing the gas sorption behavior of thin polymer films in a temperature controlled pressurized environment (up to 50 bar). The piezoelectric quartz crystal is driven by a frequency controlled AC voltage. Mass changes of the oscillating system result in a frequency shift and changes of the conductance is monitored by a network analyzer and calibrated based on the Sauerbrey equation. The study aims for the characterization of long-term behavior and physical aging of high-performance polymers for gas separation membranes - such as polyimides and polymers of intrinsic microporosity (PIMs) and respective nanocomposites. Especially the differences of the behavior of thin films compared to films with thicknesses up to 100 $\mu$m as well as nanofiller induced-effects have to be investigated.

CPP 43.11 Wed 10:00 Poster A

**MUSIC mode AFM imaging of polystyrene-grafted functionalized graphene oxide** — •Martin Dehnert[1], Eike-Christian Spitzner[1], Fabian Beckert[2], Christian Friedrich[2], and Robert Magerle[1] — [1]Chemische Physik, Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Germany — [2]Freiburger Material Forschungszentrum, Albert-Ludwigs-Universität, Freiburg, Germany

We investigate the surface morphology and the nanomechanical properties of organophilic stearylamine-modified graphene oxide (Stearyl-GO) sheets and a polystyrene-grafted functionalized graphene oxide (PS-g-FG) [1] using atomic force microscopy (AFM) operated in multi-set point intermittent contact (MUSIC) mode and force spectroscopy mode. This allows for depth-resolved mapping of the nanomechanical properties of the top surface layer of the functionalized graphene oxide (GO) sheets. On Stearyl-GO, we can distinguish areas of hydrophilic GO from hydrophobic stearylamine functionalized grafted areas. Exposure of PS-g-FG to chloroform vapor causes a selective-swelling and therefore a softening of the organic components stearyl and PS. This allows imaging the shape of the GO sheets embedded within the PS envelope. The GO sheets are folded and buckled in the PS envelope. The combination of swelling and MUSIC mode AFM imaging provides a detailed insight into the microstructure of functionalized GO sheets.

[1] Beckert F. et al.; Macromolecules, 2013, 46, 5488-5496

CPP 43.12 Wed 10:00 Poster A

**Drug Carriers based on HPMA Nanoparticles: Molar Mass and Buffer Type** — •Bart-Jan Niebuur[1], Natalya Vishnevetskaya[1], Ekaterina Lomkova[2], Petr Chytil[2], Sergey Filippov[2], and Christine M. Papadakis[1] — [1]Fachgebiet Physik weicher Materie, Physik-Department TU München, Garching — [2]Institute of Macromolecular Chemistry, Prague, Czech Republic

A promising way to achieve site-specifc delivery of anticancer agents is using the enhanced permeation and retention (EPR) effect of N-(2-hydroxypropyl) methacry-lamide (HPMA) nanoparticles containing the drug doxorubicin (Dox) [1]. The present research in this field focuses on exploration of the particle structure and tuning of their properties. Recently, addition of different types of cholesterol and degradation of the linkage is used to tune the size and stability of these nanoparticles in dependence on pH [1].

The aim of the present study is to investigate the influence of molar mass of the HPMA backbone. Using fluorescence correlation spectroscopy (FCS), the size of the nanoparticles with and without Dox as well as the critical micelle concentration (CMC) are determined in a phosphate buffer. Investigation of the polymers containing Dox is challenging because of its broad own fluorescence emission. Moreover, more realistic environments are investigated. For instance, the conditions inside the bloodstream can be mimicked using serum.

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

CPP 43.13 Wed 10:00 Poster A

**Metal Nanoparticle Growth on Model Homopolymer Thin Films** — •Vivian Waclawek[1], Matthias Schwartzkopf[2], Gonzalo Santoro[2], Johannes F.H. Risch[2], Shun Yu[3], Torsten Boese[2], Paul Staniec[4], Nick J. Terrill[4], and Stephan V. Roth[1] — [1]University of Hamburg, Luruper Chaussee 149, 22761 Hamburg — [2]DESY, Notkestr. 85, 22607 Hamburg — [3]KTH, Teknikringen 56-58, 10044 Stockholm — [4]DLS, Harwell Science and Innovation Campus, Didcot, Oxfordshire OX11 0QX

Nanostructured noble metal films on polymer layers are of fundamental importance in the field of organic electronics. Moreover, such material combinations have recently gained importance for stabilizing thin polymer films. We combine sputter deposition with grazing incidence X-ray scattering (GISAXS) to investigate in-situ [1-3] the growth kinetics of Au on polymethylmethacrylate. We analyze quantitatively the metal nanoparticle layer growth and compare our results with the metal layer structure on different model homopolymer films [4]. [1] Schwartzkopf et al., Nanoscale 5, 5053 (2013). [2] Yu et al., J. Phys. Chem. Lett. 4, 3170 (2013). [3] Santoro et al., Appl. Phys. Lett. 104, 243107 (2014). [4] Roth et al., Appl. Phys. Lett. 88, 021910 (2006).

CPP 43.14 Wed 10:00 Poster A

**Nanocomposites in High-Voltage Applications** — •Stefan O. Huber[1], Annika Rempe[2], Bruno Jakobi[3], Juriy Pachin[2], Matthias Grübel[3], Johannes Seiler[2], Josef Kindersberger[2], Bernhard Rieger[3], and Gerald J. Schneider[1] — [1]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science & Institute of Complex Systems, 52425 Jülich, Germany — [2]Department of Electrical, Electronic and Computer Engineering, Institute for High Voltage Engineering and Switchgear Technology Arcisstr. 21, 80333 Munich, Germany — [3]WACKER-Chair of Macromolecular Chemistry, Lichtenbergstr. 4, 85748 Garching, Germany

Polymer based nanocomposites may exhibit enhanced electrical insulating properties. If we add silica nanoparticles to polydimethylsiloxane, we can see in the high voltage arc resistance test that the silica nanoparticles improve the material behavior.

Our poster aims to identify the origin of the increased arc resistance in silica nanocomposites and the dependence on different parameters such as the silica-volume-fraction, the molecular mass of the polymer and in changing the modification of the nanoparticles.

We produce silica nanocomposites and by different measurements, e.g. SAXS and SANS, we characterize the microscopic behavior. From these results we want to find a model to describe the macroscopic behavior, i.e. the resistance to high voltage arcing.

CPP 43.15 Wed 10:00 Poster A

**Morphology of nanocomposite copolymer electrolytes for Li+/polymer batteries** — •Konstantinos N. Raftopoulos, Majid Rasool, Ezzeldin Metwalli, Peter Müller-Buschbaum, and Christine M. Papadakis — TU München, Physik-Department, Fachgebiet Physik weicher Materie/LS Funktionelle Materialien, Garching

Long scale, effective transition to green energy and wide penetration of electric and hybrid cars, demand for batteries with high energy and power density, good mechanical stability, as well as impact and temperature resistance. Of crucial importance for the power density and the mechanical stability is the electrolyte component. Poly(ethylene oxide) (PEO) has proven itself as a reliable electrolyte, but it has two significant drawbacks: 1) Its crystallinity, while providing some stability, acts as a barrier to the mobility of the Li cations. 2) It lacks adequate dimensional stability, especially if mixed with Li+ salts. We use a block copolymer of PEO with polystyrene (PS) in order to provide dimensional stability, and we add SiO2 nanoparticles to further enhance mechanical stability and suppress crystallinity. The morphology of the system is studied by X-ray scattering diffraction covering a large q-range, corresponding to multiple length scales, in order to study microphase separation and crystallinity.

CPP 43.16 Wed 10:00 Poster A

**Growth and disintegration of silver nanowires in tubular J-aggregates** — •Egon Steeg, Frank Polzer, Holm Kirmse, Yan Qiao, Jürgen P. Rabe, and Stefan Kirstein — Institut für Physik, Humboldt-Universität zu Berlin

The reduction of AgNO3 in the presence of tubular J-aggregates is used to prepare silver nanowires with 7 nm in diameter and lengths exceeding micrometers [1]. Here, we report on the influence of chloride ions on growth and dissolving of the wires. In presence of oxygen and a ligand the chloride ions are able to etch silver nanostructures by oxidizing neutral silver atoms back to ions [2]. This oxidative etching is more effective along defect zones than on defect free single crystals. Silver nanowires grown in the template structures are dissolved by addition of NaCl by this process and the silver is converted into AgCl while the tubular template is conserved. The dissolution of the Ag nanowires is explained by their structure which shows multiple twin boundaries. The transport of the oxidized Ag atoms is explained by transport across the tubular wall.

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

[2] Y. Zheng et al., Chem. Mater. 2014, 26, 22-33

CPP 43.17 Wed 10:00 Poster A

**Adsorption of small polar and non-polar molecules on silica-nanoparticles** — •Christina Ballnus, Sandra Katerndahl, Jan Meyer, and Reinhard Hentschke — Bergische Universität, 42279 Wuppertal, Germany

A technically important application of nano particles is their use as filler materials in rubber compounds, e.g. in the tire industry. The latter employs both soot and silica, where silica is boosted by recent EU regulations for new tires aimed at improved wet grip, rolling resistance and noise reduction. The mechanical properties of filled rubber materials are very significantly affected by the interaction of the filler with the polymer matrix. Using computer simulations based on the Metropolis Monte Carlo technique in conjunction with the charge equilibration method, we have studied the adsorption of small molecules relevant to the above industry on silica nano particles at different temperatures. We obtain the site energy distribution depending on the nano particle's surface structure and size. This we compare to experimentally obtained adsorption energy distributions. We discuss how these results may be used in simulations aimed at the prediction of dynamic moduli of silica filled rubber.

CPP 43.18 Wed 10:00 Poster A

**SAXS and NEXAFS characterization of dispersions with magnetic nanoparticles (ferrofluids)** — •Christian Gollwitzer[1], Raul Garcia Diez[1], Michael Krumrey[1], and Norbert Buske[2] — [1]Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, 10587 Berlin, Germany — [2]MagneticFluids, Berlin, Köpenicker Landstrasse 203, 12437 Berlin, Germany

Ferrofluids contain magnetic nanoparticles (like magnetite or maghemite) with superparamagnetic properties [1]. Aqueous ferrofluids with different crystal sizes between 5 nm and 10 nm (TEM) and hydrodynamic diameters between 20 nm and 200 nm (DLS) were prepared. On the one hand, the particles were electrostatically stabilized towards aggregation showing a high positive zeta potential. On the other hand, the particles were covered with fruit acids (i.e. citrate) indicating a negative zeta potential at a neutral pH value.

SAXS and NEXAFS measurements were carried out at the four-crystal monochromator (FCM) beamline of PTB at the synchrotron radiation facility BESSY II in Berlin to determine the mean size and size distribution of the primary particles, the size and fractal dimension of the agglomerates and the oxidization state of the nanoparticles. It was found, that the used ferrofluids are stable for at least several months from preparation.

[1] Rosensweig, R. 1987 Magnetic fluids. *Ann. Rev. Fluid Mech.* **19**, 437–463

CPP 43.19 Wed 10:00 Poster A

**Modeling of the phase separation behavior of nanocomposites from blockcopolymers and nanoparticles in thin films - Comparing theoretical and experimental results** — •Peter Friedel, Doris Pospiech, Dieter Jehnichen, Astrid Drechsler, Petra Uhlmann, and Andriy Horechyy — Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden

Thin films from nanocomposites containing polymer blends or blockcopolymers and nanoparticles allow manyfold applications in the generation of spezific surface structures with tailormade properties. Theoretically considered, these are three component systems with specific periodic boundary conditions. The resulting three component spinodal hypersurfaces calculated by meanfield calculations makes one able to guess the symmetry of the microphase separated structures and the distribution of the nanoparticles within the thin films. The theoretical results of two different specific copolymer systems should be compared with experimental findings. Firstly, a system containing a fixed bottom PNiPAAM layer including an dense layer of hydrophized $Fe_3O_4$ nanoparticles and an additional top layer with different polymers (containing either PMMA, P2VP or PS) was investigated as a example for polymer blend/nanoparticle composite. Secondly, a system with a PMMA-PPMA diblock copolymer including Au nanoparticles or $Fe_3O_4$ nanoparticles was investigated as an example for diblock copolymer/nanoparticle composite.

CPP 43.20 Wed 10:00 Poster A

**Periodic plasmonic nanoparticle arrays with controllable interparticle distances and plasmon resonance coupling** — •Kirsten Volk and Matthias Karg — Physical Chemistry I, University of Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany

Surface plasmons (SPs) are light induced collective oscillations of the electron liquid in respect to the crystal lattice at a metamaterial-dielectric interface with permittivities of different signs. When employing nanoparticles with a size smaller than the sink depth, optical fields can penetrate its entire volume and drive localized surface plasmon oscillations. The plasmon resonance wavelength of metallic nanoparticles is highly dependent on the size, shape and the material of the nanoparticle. Additionally the localized surface plasmon resonance (LSPR) is sensitive to the dielectric environment and the interparticle distance in nanoparticle arrays. Varying these two parameters significant changes of the optical properties of the system due to coupling can be achieved.

In this contribution we show how to make use of the dielectric environment and interparticle distance dependence of LSPRs to create functional materials with tailored optical properties. As particular building blocks we employed silver nanoparticles, which are coated by a polymer shell. The particles are then self-assembled into highly ordered hexagonally packed monolayers by a floatation approach. The interparticle distances can be exactly tuned by the dwell-time of the particles at the liquid-air interface. By placing the monolayers on substrates with high refractive indices the optical properties of the system can be further enhanced.

CPP 43.21 Wed 10:00 Poster A

**Charge Storage in $\beta$-$FeSi_2$ Nanoparticles** — Jens Theis[1], •Sebastian Küpper[1], Robert Bywalez[2], Hartmut Wiggers[2], and Axel Lorke[1] — [1]Fakultät für Physik and CENIDE, Universität Duisburg-Essen — [2]Institut 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 $\beta$-$FeSi_2$ nanoparticle layers. 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. Lateral, interdigitated capacitor structures were fabricated on thermally grown silicon dioxide and covered by $FeSi_2$ particles by drop or spin casting. The $FeSi_2$-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 around 1 V. The devices are robust and exhibit long term stability under ambient conditions. The specific capacitance is strongly dependent on the air humidity. It 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. An isotope effect can be observed by using heavy water vapour.

CPP 43.22 Wed 10:00 Poster A

**Influence of additives on the structure of CTAB and its role in gold nanoparticle formation** — •Tilo Schmutzler, Torben Schindler, Martin Schmiele, and Tobias Unruh — Friedrich-Alexander-University Erlangen-Nuernberg, Chair for Crystallography and Structural Physics, Staudtstrasse 3, 91058 Erlangen, Germany.

Au nanoparticles (NPs) have been the subject of widespread research in the last two decades. Therefore, numerous studies dealing with the synthesis leading to exact shape and size control were made. Applications are expected in biological imaging, drug delivery and photothermapeutics.[1]

The common wet chemical synthesis of anisotropic Au NPs is the seed-mediated growth synthesis route.[1] Therefore small seed particles are used to grow nanorods in a solution of CTAB (Cetyltrimethylammonium bromide) as structure directing agent.

The behaviour of CTAB in solution and so the influence on the final Au NP formation can be influenced by additives like alcohols or inorganic salts. Increasing concentrations of KBr for example lead to a higher repulsion of the micelles which was investigated by small angle X-ray and neutron scattering (SAXS, SANS) whereas UV-Vis spectroscopy revealed a slower formation kinetic of the Au NPs in KBr containing CTAB solutions. The characterization of the final Au NPs via SAXS and transmission electron microscopy (TEM) show systematic variations of the particle dimensions.

[1] C.J. Murphy et al., J. Phys. Chem B. 2005, 109, 13857-13870.

CPP 43.23 Wed 10:00 Poster A

**Effective Interaction between globular, multivalent target-inhibitor-systems** — •Susanne Liese[1], Jonathan Vonnemann[2], Daniel Lauster[3], Sumati Bathia[2], Andreas Herrmann[3], Roland R. Netz[2], and Rainer Haag[1] — [1]Freie Universität Berlin, Institut für theoretische Physik — [2]Freie Universität Berlin, Institut für Chemie und Biochemie — [3]Humboldt Universität zu Berlin, Institut für Biologie

Multivalency is an important design principle in nature. It is based on the simultaneous binding of several relatively weak binding partners, in order to strengthen the over-all interaction[1]. In our project we focus in on the interaction of globular, multivalent target-inhibitor-systems, as they are found in virus-inhibition-assays[2]. In these systems the target/inhibitor is evenly covered with receptor-/ligand-binding sites. The resulting interaction is influence by the collective binding of multiple receptor-ligand-pairs as well as by geometric shielding due to the extended size of target and inhibitor. We use a combination of coarse grained simulations and analytical methods to study the influence of the particle size, receptor/ligand-density and geometric shielding on the effective binding constant. [1] M. Mammen, S. Choi, G. M. Whitesides, Angew. Chem. Int. Ed. 1998, 37, 2754-2794 [2] I .Papp, C. Sieben, A.L. Sisson, J. Kostka, C. Böttcher, K. Ludwig, A. Herrmann, R. Haag, ChemBioChem 2011,12,887-895

CPP 43.24 Wed 10:00 Poster A

**SPONTANE TRANSFORMATION VON POLYELEKTROLYTSTABILISIERTEN SILBERNANOPRISMEN DURCH INTERAKTION MIT KSCN** — •Andrea Knauer und J. Michael Köhler — Technische Universität Ilmenau, Fak. Mat. Nat., Inst. f. Chemie und Biotechnologie, Gustav-Kirchhoffstr. 1, 98693 Ilmenau

Die Reaktion von kolloidalen Silbernanoprismen mit Rhodanidionen resultiert in einer spontanen Transformation der flachen, lateral ausgedehnten Nanoprismen in kompakte, sphärische Nanopartikel. Diese Reaktion kann nicht durch ein einfaches Ätzen der Dreiecksspitzen erklärt werden, wie es vielfach in der Literatur in Bezug auf die Reaktion mit bspw. Halogenidionen beschrieben wird. Unter beschriebenen Reaktionsbedingungen werden bei der spektralphotometrischen in-situ Überwachung isosbestische Punkte beobachtet, die darauf hinweisen, dass die Formumwandlung von einer Spezies in die andere auf direktem Weg, ohne Ausbildung von Intermediaten, geschieht. Die beobachteten Reaktionskinetiken des Umwandlungsprozesses können mithilfe eines Ansatzes der molekularen Konversion besser beschrieben werden als durch einen Prozess mit stufenweisem Transport von Material. Die Interpretation der Befunde hat hohe Signifikanz bezüglich des allgemeinen Verständnisses von formanisotropen Edelmetallnanopartikeln: Die Silber-Nanodreiecksprismen werden durch ihre spezifischen elektronischen Eigenschaften und der Interaktion mit einem oder wenigen

Polyelektrolytmolekülen stabilisiert und erscheinen eher als molekularanaloges System statt als kleine Festkörper.

CPP 43.25 Wed 10:00 Poster A

**Specific detection of molecules with NanoSPR** — •Sirin Celiksoy[1], Rubén Ahijado-Guzmán[1], Andreas Henkel[1], Janak Prasad[1,2], Christina Rosman[1], Germán Rivas[3], and Carsten Sönnichsen[1] — [1]Institute of Physikal Chemistry, University of Mainz, Germany — [2]Graduate School Materials Science in Mainz, University of Mainz, Germany — [3]Centro de Invesitigaciones Biológicas, Madrid, Spain

Nanoparticles hold potential to be used in multiplexed, inexpensive, fast medical diagnostic assays, e.g. for the identification of novel influenza strains. Common approaches for parallel analyte detection in small liquid samples link specific receptor molecules to spectrally encoded markers, thus limiting the number of targets in a parallel assay to a few dozen. Micro-spot arrays where targets bind in pre-defined positions could overcome these limitations. However, current multiplexed detection schemes are too complex, slow and/or expensive for routine use in the point-of-care environment. We show a new approach to detect multiple analytes simultaneously in a microfluidic flow cell using randomly deposited gold nanorods. Each nanorod responds with a spectral shift of its plasmon resonance specifically to one target, acting effectively as a NanoSPR device. Here, we demonstrate the feasibility of the concept, its sensitivity in the nanomolar range, sensor reusability over consecutive cycles, and the potential for up-scaling the concept. Our technique has the potential to simplify multiplexed detection and substantially reduce the costs of production, especially if combined with advanced nanofabrication methods.

CPP 43.26 Wed 10:00 Poster A

**Energy transfer characteristics of Mn doped CdS/ZnS quantum dots** — Uwe Kaiser[1], •Mikko Wilhelm[1], Johannes Röder[1], Nadeem Sabir[1], Lorenz Maximilian Schneider[1], Pablo del Pino[2], Carolina Carrillo-Carrion[1], Wolfgang Parak[1], and Wolfram Heimbrodt[1] — [1]Department of Physics, Philipps University Marburg, Germany — [2]CIC Biomagune, San Sebastian, Spain

Core shell CdS/ZnS quantum dots (QDs) doped with manganese in the ZnS shell are investigated. Photoluminescence spectra show the successful doping of the ZnS shell by the identification of the typical Mn luminescence band around 580nm. Time resolved measurements confirm this additionally by determination of the long lifetime (2ms) for this spin forbidden transition. By doping the CdS/ZnS QDs we obtain a system with two very distinct luminescence bands around 450nm from the CdS core and around 580nm from the manganese ions. The energy transfer between these two luminescence centers is not only determined by the spectral position of both bands but additionally by the interface between CdS and ZnS within the QD. The results lead furthermore to the conclusion that the low energetic Mn state cannot only act as acceptor for the high energetic CdS transition, but vice versa also as donor. This leads to an enhanced CdS lifetime from hundreds of ns without Mn to several ms in the case of Mn doping. Measurements of Mn doped QDs and QDs additionally functionalized by dye molecules also show a lifetime of the dye in the ms range, due to energy transfer from the excited Mn.

## CPP 44: P9: Crystallization, Nucleation and Self Assembly

Time: Wednesday 10:00–13:00 Location: Poster A

CPP 44.1 Wed 10:00 Poster A

**Experimentelles zum zum Beleg der Kettenfaltung in Lamellen bei massivem HDPE** — •Heinz Preuss — 31785 Hameln

Es werden die experimentellen Verfahrensschritte dargestellt, die zum elektronenmikroskopischen Nachweis der Existenz von Lamellen als relativ selbständige Strukturformen in massivem Niederdruckpolyethylen (HDPE) geführt und Belege für die Realität des Kettenfaltungsmodells gebracht haben. Dabei handelt es sich um einen Oberflächenabriss mit einer Metallmatrize aus aufgedampftem Gold mit galvanischer Verstärkung durch Kupfer und Schrägbedampfung (30 Grad) mit Kohlenstoff aus einem Lichtbogen. Ein weiterer Beleg ergibt sich mit der im TEM direkt beobachteten faktisch übergangslosen Umwandlung von Lamellen in Fasern beim Zerreißen einer dünnen PE-Haut die beim Kristallisieren aus einer Lösung mit Xylol auf heißem Wasser entstanden ist. (H.H.W.Preuß, Dissertation. Leipzig 1963; Plaste und Kautschuk 22. Jg. Heft 12/1975, S. 958 ff.)

CPP 44.2 Wed 10:00 Poster A

**Crystallization of nearly hard spheres under shear** — •David Richard and Thomas Speck — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany

Rare events are an outstanding challenge in modern computational science: protein folding, chemical reactions, nucleation during phase transitions. During the last decades, advanced numerical schemes have been developed to study the transition between two states A and B. In liquid and colloidal systems, Umbrella Sampling and Forward Flux Sampling have been shown to be in good agreement with 'brute force' Molecular Dynamics simulations for crystallization rates [1][2]. However, the nucleation process under external forces like electric fields or flow remains poorly understood. Therefore, rare event sampling techniques have to be extended for systems driven out of equilibrium. We present results for crystallization rates in a liquid of nearly hard spheres under a weak linear shear flow using straightforward Molecular Dynamics and Forward Flux Sampling.

[1] Crystal nucleation of hard spheres using molecular dynamics, umbrella sampling, and forward flux sampling: A comparison of simulation techniques. L.Filion, M. Hermes. R. Ni, and M. Dijkstra. The Journal of Chemical Physics 133 (2010)

[2]Simulation of nucleation in almost hard-spheres colloids: The discrepancy between experiment and simulation persists. L.Filion, R.Ni, D.Frenkel, and M.Dijkstra. The Journal of Chemical Physics 134 (2011).

CPP 44.3 Wed 10:00 Poster A

**Direct Observation of Crystallization through Surface Wrinkling in Polymer Thin Film** — •Peng Zhang[1], Gonzalo Santoro[1], Sarathlal K. Vayalil[1], Ezzeldin Metwalli[2], Peter Müller-Buschbaum[2], Tianbai He[3], and Stephan V. Roth[1] — [1]Deutsches Elektronen Synchrotron, Notkestr. 85, 22607 Hamburg, Germany — [2]Technische Universität München, Physik-Department, LS E13, James-Franck-Str.1, 85747 Garching, Germany — [3]State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, China

Polymer crystallization is a well concerned and yet unclear phase transition from amorphous coils to well organized nanoscale lamellae. Among the research areas of interest are fundamental issues relating to the early stages of polymer crystallization.1,2 Here we explore the structural transition at the early stages of ordering towards crystallization in diblock copolymer thin films. The structure change at early stages of crystallization is unraveled from a perspective of cooling induced density change. The diblock copolymer thin film offers a well confined crystallization case where the density change can be linked with the lateral molecular diffusion. Moreover, the cooling induced surface wrinkling promotes the nucleation and crystal growth in polymer. These findings provide us a new perspective to understand the whole scenario of polymer crystallization. [1] Strobl, G. Eur. Phys. J. E 3, 165 (2000); [2]Cheng, S. Phase Transitions in Polymers: The Role of Metastable States; Elsevier Science: Amsterdam, 2008.

CPP 44.4 Wed 10:00 Poster A

**Ultra-fast scanning calorimetry of polymers implying cooling up to 10,000,000 K/s** — •Evgeny Zhuravlev[1], Sander van Herwaarden[2], Vadlamudi Madhavi[3], and Christoph Schick[1] — [1]University of Rostock, Rostock, Germany — [2]Xensor Integration, Delft, Netherlands — [3]ExxonMobil Research & Engineering Company, Annandale, NJ, USA

The complexity of polymer crystallization is often demonstrated on the example of simple polyethylene molecule. But it's simplicity can become a disadvantage. The simple molecules can crystallize so fast, that few to none experimental technique is able to follow it. Especially in the region of homogeneous nucleation - approaching a glass transition temperature from the melt - a point of controversy in polymer science. Bypassing glass transition, avoiding crystallization, for the purpose of it's further investigation at any desired temperature has been challenged by ultra-fast scanning calorimetry since years. Recent achievements has extended maximum possible cooling rate of nanogram sample up 10,000,000 K/s. Further reheating of this sample at 1,000,000 K/s, showing the glass transition, cold crystallization and melting of quenched polyethylene, is reported.

CPP 44.5 Wed 10:00 Poster A

**Neutron and X-ray Scattering Studies on Nanoconfined Liquids and Solids** — •Tommy Hofmann[1], Dirk Wallacher[1], and Patrick Huber[2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Str. 15, 12489 Berlin, Germany — [2]Hamburg University of Technology, Eißendorfer Straße 42, 21073 Hamburg, Germany

Condensed matter confined on nanometer-sized length scales exhibits different structural and dynamical properties than its bulk counterparts. Surface interactions and pure confinement effects alter the characteristics of matter as the system size is reduced in an intriguing way. On this poster, we discuss how confinement in tubular, aligned channels a few nanometer across affects the mesoscopic arrangement of liquids and the crystal structure and texture of solidified condensates. We present x-ray as well as neutron scattering studies on pore-confined deuterium, nitrogen, oxygen and various n-alkanes.

CPP 44.6 Wed 10:00 Poster A

**Enhanced phase purity in sexithiophene thin films through laser illumination** — •Linus Pithan[1], Caterina Cocchi[1,2], Hannes Zschiesche[1], Christopher Weber[1], Anton Zykov[1], Sebastian Bommel[1,3], Peter Schäfer[1], Steven Leake[4], Claudia Draxl[1,2], and Stefan Kowarik[1] — [1]Instiut für Physik, Humboldt Universität zu Berlin — [2]IRIS Adlershof, HU Berlin — [3]DESY, Hamburg — [4]Swiss Light Source, PSI, present address: ESRF, France

We study the influence of light on the phase coexistence in $\alpha$-sexithiophene (6T) thin films. We focus on vacuum deposited films grown on potassium chloride (KCl) that exhibit a bimodal growth with two co-existing crystal phases, the low-temperature (LT) and high-temperature (HT) 6T polymorphs. We find that laser illumination ($532\,nm$, $1.5\,W/cm^2$) during growth suppresses the formation of HT crystallites, thus the phase purity is enhanced compared to the bimodal growth without light. To understand the mechanism behind this optical control, we use *in situ* x-ray diffraction, atomic force microscopy (AFM), optical absorption measurements, as well as first-principles calculations for the optical absorption spectra of the HT and LT phase. We deduce that the phase purification is due to optical heating of the molecular film and lower cohesive energy of the HT phase compared to the LT phase. This finding demonstrates that light can serve as an additional control parameter in molecular crystal growth to optimize the structural quality of molecular thin films.

CPP 44.7 Wed 10:00 Poster A

**A soft, bilayer phase in nanoparticle-doped n-CB homologues** — •Alexander Lorenz[1], Dena M. Agra-Kooijman[2], Dean R. Evans[3], Heinz-S. Kitzerow[4], and Satyendra Kumar[2] — [1]Stranski-Laboratorium, Sek. TC 9, Technische Universität Berlin, Str. des 17. Juni 124, 10623 Berlin, Germany — [2]Department of Physics, Kent State University, Kent, Ohio 44242, USA — [3]Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson Air Force Base, Ohio 45433, USA — [4]Department of Chemistry, Universität Paderborn, Warburger Straße 100, 33098 Paderborn, Germany

Several homologues of the n-alkyl-cyanobiphenyl series were doped with BaTiO3 nanoparticles (dispersed in heptane) [1,2]. Synchrotron x-ray scattering experiments of the doped n-pentyl-cyanobiphenyl and n-octyl-cyanobiphenyl samples revealed nine orders of a primary Bragg reflection, respectively [2]. These scattering signals were caused by a soft, one-dimensional multilayer structure and were not present in the neat substances. The scattering signals were used to calculate the electron density profiles inside the multilayers by Fourier analysis; the multilayers were found to be one-dimensional, multilayered, smectic nanostructures in each case. In conclusion, doping clearly induced a novel, self-assembled nanostructure in which the rigid aromatic part, and not the overall length, of the molecules defined the layer spacing. A. Lorenz et al. Physical Review E 86, 051704 (2012). A. Lorenz et al., Physical Review E 88, 062505 (2013).

CPP 44.8 Wed 10:00 Poster A

**Reversible switching between self-assembled nanoribbons and nanotubes** — •Asad Jamal[1,2], Philippe Mesini[3], and Günter Reiter[1,2] — [1]Physikalisches Institut und — [2]Freiburger Materialforschungszentrum, Albert-Ludwigs-Universität Freiburg, 79104 Freiburg, Germany — [3]Institut Charles Sadron, 23 rue du Loess BP 84047, 67034 Strasbourg Cedex 2, France

Depending on the quality of the solvent, achiral 3,5-bis(5-hexylcarbamoyl-pentyloxy)-benzoic acid decyl ester (BHPB-10) molecules were self-assembles into nanotubes of about 10 nanometer in width and nanoribbons with a diameter of ca. 40 nanometer, both having several micrometers in length. In solvents weakly interacting with BHPB-10 like cyclohexane nanotubes were formed while in solvents with comparatively strong molecule-solvent interactions like cyclohexanone nanoribbons were created. Interestingly, annealing nanoribbons in the vapor of cyclohexane allowed to switch them to nanotubes. Moreover, changing the solvent from cyclohexane to cyclohexanone switched nanotubes back into nanoribbons. Atomic force microscopy studies indicated that nanoribbons transited through helical twisted nanosheets into tubular structures. We relate the nanotube formation to hydrogen-bonds among the BHPB-10 molecules which are not possible in cyclohexanone.

CPP 44.9 Wed 10:00 Poster A

**Breath figure template: an effective fabrication technique for large area micro-lenses array** — •farid farajollahi, othmar marti, and masoud amirkhani — Institute of Experimental Physics, University of Ulm, 89069 Ulm, Germany

Condensation of water on polymeric solution can produce a micro pattern by using of breath figure technique. The hexagonal arrangement of micro droplets of water does imprint pore structure on the surface of the polymer after evaporation of all liquid. The pore size and arrangement can be adjusted by changing the concentration of polymer and solution composition. The microstructure on polymer film is used as a template for fabricating micro-lens array by molding technique. Polydimethylsiloxan (PDMS) can be cast on the template to make a replica version of micro-pattern, which creates convex micro lenses with hexagonal arrangement. The shape, focal length and the filling factor of micro-lenses are measured by optical microscope and SEM. This method provides a fast and simple way to fabrication of hexagonal micro-lens structure.

CPP 44.10 Wed 10:00 Poster A

**Applying breath figure technique for the fabrication of porous film using various solvents** — •mandeep singh, farid farajollahi, othmar marti, and masoud amirkhani — Institute of Experimental Physics, University of Ulm, 89069 Ulm, Germany

Elsewhere, has been shown that using the breath figure technique and adding the appropriate amount of alcohol to the solution of polymer/chloroform one can fabricate a well order honeycomb structure on the surface of polymer film. In this study, we show how different solvent may effect on the structure and size of pores on the surface. We employed several organic solvent from different solvent family and with various evaporation rates while the polymer (polystyrene) and alcohol (methanol) remain same for all samples. This study enables us to formulate underling important parameter, which governs the formation of porous structure.

CPP 44.11 Wed 10:00 Poster A

**Optical waveguiding and anisotropic behavior of large single crystal of thiophene-based oligomers** — •Sajedeh Motamen[1], Yingying Wang[1], Jean-Pierre Malval[2], Thibaut Jarrosson[3], Françoise Serein-Spirau[3], Laurent Simon[2], and Günter Reiter[1] — [1]Physikalisches Institut, Albert-Ludwigs-Universität, 79104 Freiburg, Germany — [2]Institut de Sciences des Materiaux de Mulhouse IS2M, 4 rue des freres Lumiere, 68093 Mulhouse, France — [3]Institut Charles Gerhardt de Montpellier, 8 Rue de lEcole Normale, 34296 Montpellier cedex 05, France

Unique properties of conjugated organic molecules are responsible for their remarkable potential as active elements in optoelectronic devices such as field-effect transistors or solar cells. For achieving high performance, ordering of these conjugated molecules within the active layer of these devices has been considered as a promising pathway. Single crystals with unique molecular orientation represent ideal model systems for the corresponding systematic studies. Here, we report the formation of large single crystals of 2,5-dialkoxy-phenylene-thienylenebased oligomers (3TBT). Compared to disordered aggregates in spin-coated thin films, single crystals exhibited a pronounced red shift in absorption and photoluminescence spectra, indicating an increase of the conjugation length. As a consequence of high molecular order, an extremely high dichroic ratio was observed. Without any external stimulation, light could travel along the long axis of the crystal over few hundreds of micrometer. We relate structural properties to this observed optical waveguiding effect, which may be of relevance in applications.

CPP 44.12 Wed 10:00 Poster A

**Atomistic simulations of oriented attachment of hematite nanoparticles** — •Henning Hörstermann, Thomas Gruhn, and Heike Emmerich — University Bayreuth, Chair of Material and Process Simulations, Bayreuth, Germany

Interactions between two hematite nanoparticles with diameters of a few nanometers are studied via molecular statics and molecular dynamics methods. We try to identify favorable crystal faces for oriented attachment by calculating the contact energies of nanoparticles attached to each other via aligned contact areas of a defined structure. We present an approach to identify the time scales on which particles approach each other and their relative orientation changes towards perfect aligment by combining information about the interaction of the particles with direct observation of the attachment process. This information can be used to formulate criteria to decide if two particles with given initial relative position and orientation will combine or disperse and if the differences in alignment can be eliminated before attachment and to estimate probabilities and rates for aggregation and oriented attachment.

CPP 44.13 Wed 10:00 Poster A

**Photonic materials from hydrogel-coated gold nanocrystals: Effect of cross-linker density, temperature and volume fraction** — •Astrid Rauh and Matthias Karg — Physical Chemsitry I, University of Bayreuth, Germany

The self-assembly of soft polymer colloids allows the preparation of photonic materials with responsive bandgap behavior. To increase the refractive index of a polymer material and thus the diffraction, the implementation of inorganic cores can be useful. We synthesized a series of single gold nanoparticle cores encapsulated in a cross-linked poly-N-isopropylacrylamide (PNIPAM) shell. To investigate the influence of the thermoresponsive hydrogel shell morphology on the crystallization behavior, the shell thickness and cross-linker density were varied. The cross-linker density influences the softness and the swelling capacity of the polymer network.

The crystallization behavior was investigated in dependence of volume fraction and temperature. We found crystalline structures with diffraction in the visible for a broad range of concentrations. A lower crosslinking density supported the crystal formation. Increasing the temperature, the volume fraction of the core-shell particles is lowered.[1] Therefore, a melting of the crystals in a certain concentration range can be achieved. Upon cooling the crystalline structures exceed the critical volume fraction and form again colloidal crystals. This indicates the reversibility of the structure formation.

[1] M. Karg, T. Hellweg, P. Mulvaney, Adv. Funct. Mater. 2011, 21, 4668-4676

## CPP 45: P10: Colloids and Complex Liquids

Time: Wednesday 10:00–13:00 Location: Poster A

CPP 45.1 Wed 10:00 Poster A

**Early stage of liquid-liquid phase separation in protein solutions studied by USAXS** — •Fajun Zhang[1], Stefano Da Vela[1], Michal Braun[1], Michael Sztucki[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]ESRF, Grenoble, France

We present new results on the early stage of liquid-liquid phase separation (LLPS) in protein-salt solutions using the improved USAXS beamline (ID2, ESRF). We use our model system of bovine serum albumin (BSA) with $YCl_3$ [1,2], which shows LLPS and a lower critical solution temperature (LCST) phase behavior and can be rationalized using an ion-activated patchy-colloid model [3]. The USAXS data of sample solutions after a temperature jump exhibit a peak that grows in intensity and shifts to lower q values with time. The characteristic length scale obtained from this scattering peak increases with time as $t^{0.3}$, which will be further discussed for different temperature jumps as well as sample compositions. The method established in this work can be used to study the arrested spinodal decomposition in protein and colloid systems covering both the correlation length and the local structure. [1] F. Zhang, et al. Phys. Rev. Lett. 101, 148101 (2008) Proteins 78, 3450-3457 (2010). [2] F. Zhang, et al. Soft Matter 8, 1313-1316 (2012) and Faraday Discuss. 159, 313-325 (2012) [3] F. Roosen-Runge, et al. Sci. Rep. 4, 7016 (2014)

CPP 45.2 Wed 10:00 Poster A

**Dynamics of a rigid particle near a deformable interface in a viscous flow** — •Abdallah Daddi-Moussa-Ider, Achim Guckenberger, and Stephan Gekle — Biofluid Simulation and Modeling, University of Bayreuth, Germany

Using computer simulations, we study the parallel motion of a rigid particle moving close to a deformable elastic membrane. We use a completed double layer boundary integral formulation to solve the Stokes equation in the limit of low Reynolds numbers. The interface deformability is treated in the linear response framework where its elastic energy is locally stored in a shear deformation and dilatation. A bending resistance has been included in order to account for the strong local curvatures. By dragging the rigid particle parallel to the elastic interface, we evaluate the drag coefficient for several distances from the surface. An elasto-hydrodynamic coupling between the flow and the wall deformation plays an important role for the particle dynamics. We find that the drag coefficient and the rotation about the axis parallel to the interface are largely dependent on the interface rigidity. We compare our numerical results for high stiffness values with the analytically exact solutions in the hard wall limit.

CPP 45.3 Wed 10:00 Poster A

**Phase Unwrapping of two-dimensional interferograms - Preparations for the DCMIX-3 experiment on board the ISS** — •Thomas Triller and Werner Köhler — Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany

The DCMIX project is an international effort to investigate diffusive transport in ternary fluid systems in the presence of a temperature gradient. In certain systems these processes are prone to gravitational instability. Therefore, experiments have been designed in a microgravity environment on board the ISS with SODI (Selectable Optical Diagnostics Instrument). SODI is a variation of a Mach-Zehnder interferometer and thus generates two-dimensional interferograms of a thermodiffusion cell. To analyse these interferograms and extract transport coefficients (e.g. the Soret coefficients of the diffusing components), the image information has to be processed with the Phase Unwrapping method. Such image processing is necessary, because the phase information $\psi(t)$ in the images is wrapped into the range $(-\pi, \pi]$: $\psi(t) = \varphi(t) + 2\pi k(t)$ with $k(t)$ an integer function. The full phase $\varphi(t)$ has to be reconstructed with proper algorithms. As preparations for the DCMIX-3 experiment (the system Water/Ethanol/Triethylene-glycol), several algorithms for Phase Unwrapping have been implemented and compared.

CPP 45.4 Wed 10:00 Poster A

**Density functional theory for the bulk phases of a colloid-polymer mixture** — •Mostafa Mortazavifar and Martin Oettel — Institut für Angewandte Physik, Uni Tübingen, Tübingen, Germany

We propose to treat gas, liquid, and crystal phases of the Asakura-Oosawa model (AO) for a colloid-polymer mixture within the framework of Fundamental Measure Theory. In AO model the polymers are an ideal gas, but colloid-colloid and colloid-polymer interactions are of hard sphere type. A new expression is derived for the excess part of the free energy. The bulk free energy and liquid-gas transition are calculated for various values of polymer reservoir packing fraction, $\eta_p^r$, and colloid-polymer size ratios, $q = \frac{2R_g}{\sigma}$; $\sigma$ is the diameter of colloid particles and $R_g$ is the gyration radius of polymers. By a self consistent full minimization scheme the free energy of the fcc solid and the solid-liquid phase transition is calculated for different values of $q$ and $\eta_p^r$. In the limit of $\eta_p^r$ to zero, the problem reduces to the pure hard sphere case. By increasing the reservoir packing fraction of polymers, the fluid-solid coexistence region broadens compared to pure hard spheres.

CPP 45.5 Wed 10:00 Poster A

**Contribution to a benchmark test on thermodiffusion in an organic ternary mixture** — •Matthias Gebhardt and Werner Köhler — Physikalisches Institut, Universität Bayreuth, D-95440 Bayreuth, Germany

The knowledge of diffusive mass transport in liquid mixtures is important for several natural and technological processes. Especially in the presence of a temperature gradient, where the local composition of a mixture is linked to an inhomogeneous temperature field. In the last decades binary mixtures were investigated in detail and a significant data base has been established. Today, experiments are going one step further and are challenging ternary mixtures. However, first results of multicomponent experiments performed by different groups and methods have shown the difficulties and complexity of this scientific subject. Furthermore, gravity can have a destabilizing effect on many of these diffusion experiments. Therefore, an international community has decided to establish benchmark values for the diffusion, thermodiffusion and Soret coefficients of the organic ternary mixture 0.8/0.1/0.1 (mass fraction) of 1,2,3,4-tetrahydronaphthalene, isobutylbenzene and n-dodecane in microgravity environment aboard the International Space Station (ISS) and on ground. We are presenting our contribution to this benchmark test by means of a two-color optical beam deflection technique.

CPP 45.6 Wed 10:00 Poster A

**Resolving high-speed colloidal dynamics beyond detector response time via two-pulse speckle contrast correlation** — •Sooheyoung Lee[1], Wonhyuk Jo[1,2], Hengsub Wi[1], Christian Gutt[3], Jan Verwohlt[3], and Geunwoo Lee[1] — [1]Korea Research Institute of Standards and Science, Daejeon, Republic of Korea — [2]Department of Physics, Soongsil University, Seoul, Republic of Korea — [3]Department Physik, Universität Siegen, Germany

We report an alternate light scattering approach to measure the intermediate scattering function and structures of colloidal suspensions by using two-pulse speckle contrast correlation analysis. By systematically controlling time-delays between two laser pulses incident on the sample, we are able to monitor transient evolution of coherent diffraction pattern, from which particle dynamics at different length and time scales are obtained simultaneously. Our result demonstrates the feasibility of utilizing a megapixel detector to achieve sufficient data statistics in a short amount of time while enabling microsecond time-resolution. Ultimately, this method provides means to measure high-speed dynamics well beyond the time response limit of a large area two-dimensional (2D) detector.

CPP 45.7 Wed 10:00 Poster A

**Increasing the bending modulus of AOT based microemulsions by the addition of polymer** — •Ann-Kathrin Grefe, Björn Kuttich, and Bernd Stühn — Experimental Condensed Matter Physics, TU Darmstadt, Germany

Being a highly versatile system, microemulsions are applied in many different fields from medical science to oil production. In order to make such implementations accessible, an extensive understanding of the interactions in microemulsions, especially in the presence of additives, is essential. Microemulsions with added polymers represent a suitable simplified model system to study these interactions.

This work focuses on the analysis of AOT based w/o microemulsions in the droplet phase, modified by the water soluble polymer polyethylene glycol (PEG). The polymer is confined to the water core of the droplets where it is expected to adsorb at the surfactant shell. Due to the adsorption the bending modulus of the shell changes, which in turn affects the phase diagram of the microemulsion.

Samples with different amounts of polymer are examined by dielectric spectroscopy to find their percolation and phase separation temperatures. Temperature resolved small angle X-ray scattering allows the determination of the water droplet sizes. In doing so, a dependence of the droplet radius on the molar ratio of water and surfactant as well as on the temperature is found and quantified. Both are significantly influenced by the presence of polymer. Combining dielectric and scattering experiments the bending modulus of the surfactant shell can be deduced and a stiffening of the shell due to the polymer is found.

CPP 45.8 Wed 10:00 Poster A

**Clusters formation of patchy particles** — •Reint Hieronimus and Andreas Heuer — Westfälische Wilhelms-Universität Münster, Institut für physikalische Chemie, Corrensstrasse 30, 48149 Münster, Germany

A system of patchy particles can aggregate in different ways to clusters. The aggregation behaviour is determined by the particle geometry and the type of patch interaction. In order to estimate the probability of finding clusters of different sizes we calculated their free energy. This was done by performing Monte-Carlo simulations in combination with thermodynamic integration. Our method is independent of the chosen potential and can be used for any particle geometry. As a verification, we compared the simulation results to analytic results for a one-dimensional system using the well-known model by Kern and Frenkel.

CPP 45.9 Wed 10:00 Poster A

**The influence of Brownian motion on sheared nanocomposites: New experimental results and a revision of Peclet-time as a characteristic time scale** — •Rick Dannert, Roland Sanctuary, and Jörg Baller — University of Luxembourg, Laboratory for the Physics of Advanced Materials, Grand-Duchy of Luxembourg

Oscillatory shear tests performed on concentrated and semi-diluted suspensions of spherical silica nanoparticles in Diglycidyl Ether of Bisphenol A (DGEBA) have revealed a low-frequency relaxation process. The latter was interpreted as Brownian stress relaxation resulting from strain-induced perturbations of the isotropic filler distribution [1]. To cover a broader concentration range we have extended the rheological investigation of the low-frequency anomaly to ultra-diluted DGEBA/silica suspensions. We illustrate that the Brownian relaxation process depends in a complex manner on the volume concentration: For very dilute systems, the relaxation frequency increases with the concentration, whereas for semi-dilute or concentrated systems, the opposite behaviour can be observed. This non-monotonic dependency of the relaxation frequency can no longer be modelled by classical Peclet frequencies. Therefore we show that modified Peclet-frequencies including a structural, concentration dependent length scale viz. the mean particle distance lead to an accurate description of the Brownian relaxation process for all concentrations.

[1] R. Dannert, R. Sanctuary, M. Thomassey, P. Elens, J.K. Krüger, J. Baller, Rheologica Acta, 53 (2014) 715-723.

CPP 45.10 Wed 10:00 Poster A

**Rheological study of anisometric pigment particle suspensions** — •Yong Geng, Alexey Eremin, and Ralf Stannarius — Otto-von-Guericke-Universität Magdeburg, FNW/IEP/ANP, Postfach 4120, 39016 Magdeburg, Germany

Rheological properties of colloidal suspensions formed by nanometer size rod-shaped pigment particles dispersed in a non-polar solvent are studied. Experiments have shown that these suspensions possess unusual properties such as liquid crystalline behaviour at high dispersant concentration, field-induced phase separation at low and intermediate concentrations, switching in electric fields, and a reversible response to the adsorbing light affecting current transients in sandwich cells.1,2 By doping with small amounts of ferrofluid these pigment dispersions can form a basis for magneto-responsive materials. A strong magneto-optical effect has been confirmed. In our studies, we demonstrate a strong shear-induced birefringence and shear thinning behaviour in pure dispersions. We also discuss the effects of magnetic fields on the rheological properties of the pigment/ferrofluid mixtures. This helped to get a deeper insight into the properties of these suspensions and understand the mechanisms of the structural changes under external field such as electric, magnetic and flow.

1. Eremin, Alexey, et al., Adv. Funct. Materials 21.3 (2011): 556-564. 2. Greasty, Robert J., et al., Phil. Trans. Roy. Soc. A 371.1988 (2013): 20120257.

CPP 45.11 Wed 10:00 Poster A

**Fundamental Measure Theory for 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.

The isotropic–nematic interfacial tension remarkably improves on earlier, only qualitatively correct predictions for director dependence and density profile [2]. For the first time we obtain a phase diagram of hard spherocylinders, including a stable smectic phase [3], which can be quantitatively compared to simulations. To verify the consitency of the different FMT approaches, we study the the phase behavior of parallel spherocylinders and the elasticity of the nematic phase analytically.

[1] H. Hansen-Goos and K. Mecke, Phys. Rev. Lett. **102**, 018302 (2009).
[2] R. Wittmann and K. Mecke, J. Chem. Phys. **140**, 104703 (2014).
[3] R. Wittmann, M. Marechal and K. Mecke, J. Chem. Phys. **141**, 064103 (2014).

CPP 45.12 Wed 10:00 Poster A

**Defect topolgies in chiral blue phases confined to mesoscopic channels** — Sergej Schlotthauer[1], •Robert Skutnik[1], Tillmann Stieger[1], and Martin Schoen[1,2] — [1]Technische Universität Berlin, Berlin, Germany — [2]North Carolina State University, Raleigh (NC), USA

Soft matter confined to volumes of nanoscopic extent constitutes an interesting class of systems. In particular a lot of work has already been invested to study confined liquid crystals. The focus of this study is the orientational order of liquid-crystals and especially their deformation. In the case of non-chiral nematic liquid crystals one immediately may think of the twisted-nematic cell where the nematic director rotates between the substrates and a quasi-cholesteric helix evolves. The more recent research focuses on confined chiral phases, e.g. cholesteric or blue phases. If the introduced substrates are separated by a distance which is not equal to a multiple of half pitches transitions between the inherent defects of blue phases may be observed. Two-dimensional confinement (i.e. circular or rectangular mesochannels) of liquid crystals has been less far studied to date. In the late 1970s and early 1980s theoretical studies focused on the orientational order of nematic phases in tubular spaces. However, to the best of our knowledge there is no systematic study of chiral phases confined in two dimensions up to date. In our study we focus on two-dimensional confinement of chiral liquid crystals where we observe a host of novel topological defects. Furthermore, the geometry of the chosen channel and its surface anchoring determines the defect structure.

CPP 45.13 Wed 10:00 Poster A

**Self-assembling nanoparticles systems: influence of particles shape and concentration** — •Elena Pyanzina — Ural Federal University, Lenin av. 51, Ekaterinburg, 620000, Russia

The process of self-assembly is a key to design and control various systems, and as such it has recently become a subject of interest in physics, chemistry and biology [M. Nakata et al., Science, 2007]. Self-assembling building blocks might be of different nature and size might also form clusters of almost arbitrary topology. In the present study we focus on one two type of building blocks: superquadrics (namely, elongated spherocylinders) and discs, that can form different type of clusters. We present the analytical model for calculation structural properties and investigate them as functions of particles shape and concentration. Our conclusions are supported by an extensive comparison of the theoretical predictions to the results of computer simulations.

## CPP 46: P11: Wetting, Micro and Nano Fluidics

Time: Wednesday 10:00–13:00 Location: Poster A

CPP 46.1 Wed 10:00 Poster A

**Enhanced microfluid mixing due to the near-surface transport of superparamagnetic bead rows** — •Dennis Holzinger and Arno Ehresmann — Department of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel

An accurate computational fluid dynamic simulation model is presented for the domain wall movement assisted transport (DOWMAT) of full superparamagnetic bead rows above a micromagnetic stripe-patterned exchange bias layer system for enhanced active mixing in a laminar flow microfluidic device using Comsol Multiphysics.[1,2] The simulation model takes into account the effect of device length scales, the diffusive properties of the diluted species and the applied movement scheme of the superparamagnetic bead rows. The results demonstrate that the maximum achievable mixing velocity strongly depends on the above stated parameters, so that the microfluidic device parameters can be specifically tailored e.g. for biosensing applications in lab-on-a-chip (LOC) devices prior to the experimental implementation.

[1] A. Ehresmann, D. Lengemann, T. Weis, A. Albrecht, J. Langfahl-Klabes, F. Goellner and D. Engel, Adv. Mater. 23, 5568 (2011)
[2] D. Holzinger, D. Lengemann, F. Goellner, D. Engel and A. Ehresmann, Appl. Phys. Lett. 100, 153504 (2012)

CPP 46.2 Wed 10:00 Poster A

**Quantifying dynamic wetting of surfactant solutions** — Franziska Henrich, Dorota Truszkowska, Hans-Jürgen Butt, and •Günter K. Auernhammer — MPI Polymer Research, Mainz, Germany

Although in recent years there have been efforts to gain better understanding on the dynamic wetting of surfactant solutions [1,2], the flow profile near the 3-phase contact line still is not entirely known. In the hydrodynamic model of the flow profile, the diffusion of surfactant to the surface plays an important role, since in this model surfactant molecules flows due to gradient of the surface tension to the new surface near the 3-phase contact line. In this contribution we present methods to determine the dynamic contact angle, the flow profile and the surfactant concentration. We discuss the characteristic changes due to different surfactants and surface structure.

[1]Fell, D. et al. Langmuir (2011): 27(6) 2112-2117
[2] Fell, D. et al. Colloid and Polymer Science (2013), 291(2) 361-366

CPP 46.3 Wed 10:00 Poster A

**Relaxation of Surface Perturbations in Thin Liquid Films as a Probe of Liquid/Substrate Interactions** — •Marco Rivetti[1], Christine Linne[1], Paul Fowler[1,2], Joshua D. McGraw[2], Thomas Salez[3], Michael Benzaquen[3], Elie Raphaël[3], Kari Dalnoki-Veress[2,3], and Oliver Bäumchen[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — [2]Department of Physics & Astronomy, McMaster University, Hamilton, Canada — [3]PCT Lab, UMR CNRS 7083 Gulliver, ESPCI ParisTech, PSL Research University, Paris, France

Perturbations of the free surface of a thin liquid film relax due to capillary forces. Flow is driven by local curvature gradients of the surface and resisted by the liquid's viscosity. For an initial non-equilibrium profile given by a step geometry, capillary leveling is shown to result in self-similar profiles. We find an excellent agreement between experimental profiles, as obtained from atomic force microscopy data, and numerical calculations. For liquid films supported by rigid substrates and in the presence of a no-slip boundary condition, this system provides a precise nano-rheological probe of the capillary velocity. For flows on small length scales, however, the interactions of liquid molecules with the substrate at the solid/liquid interface become important. We show that the capillary levelling is sensitive to the slip boundary condition at the solid/liquid interface. Thin film models comprising hydrodynamic slip enable a quantification of the slip length. Aside from friction, energy can also be dissipated through the elastic deformation of the substrate, which we will discuss in detail.

CPP 46.4 Wed 10:00 Poster A

**Liquid-liquid dewetting** — •Stefan Bommer[1], Nikolas Becker[1], Ralf Seemann[1], Sebastian Jachalski[2], Dirk Peschka[2] und Barbara Wagner[2] — [1]Universität des Saarlandes — [2]TU Berlin

The transient morphologies towards equilibrium of liquid droplets dewetting on another liquid as well as the dynamics of dewetting rims are considered experimentally and theoretically. As liquids short chained polystyrene and polymethylmethacrylate are used which are glassy at room temperature and which can be considered as Newtonian liquids well above their glass transition temperatures. The liquid/air interfaces are imaged in situ by scanning force microscopy whereas the liquid/liquid interface is imaged after solidifying the sample and removing the dewetting polystyrene. The transient shapes are modeled by lubrication approximation and Stokes model using the relevant experimental parameters like the ratio of film thicknesses, the viscosity rations, the ratio of the surface tensions of the liquid/air and the liquid/liquid interface, and the contact angles. A remarkably independence of the transient shapes on the start conditions was found theoretically for sufficiently 'mature' droplets which allow for a quantitative comparison with experimental droplet morphologies. Carrying on from this successful comparison, we also investigate the shape and dynamics of dewetting rim profiles.

CPP 46.5 Wed 10:00 Poster A

**Super Liquid-Repellency: Mechanical Robustness vs. Repellency** — •Maxime Paven, Frank Schellenberger, Michael Kappl, Doris Vollmer, and Hans-Jürgen Butt — Max Planck Institute for Polymer Research, Mainz, Germany

So-called super liquid-repellent - or superamphiphobic - layers cannot only repel water but also many low surface tension liquids like soap solutions, hexadecane or organic compounds. Superamphiphobic surfaces have various potential applications ranging from self-cleaning solar cells to anti-biofouling medical devices. Next to a simple fabrication method, the mechanical robustness and durability of these layers is mandatory. Recently, our group developed a facile surface preparation technique to fabricate superamphiphobic layers, based on a fractal-like network of hydrophobized nanometer sized silica spheres. Considering the surface morphology, a simplified theoretical approach predicts, that the mechanical robustness and liquid repellency cannot be increased at the same time. We studied the interplay between mechanical robustness and repellency experimentally. By tuning the reaction parameters, surfaces with varying mechanical and wetting properties were obtained. The elastic and plastic responses of these layers were investigated by atomic force microscopy (AFM). Therefore, a colloid was attached to a cantilever and force versus distance curves were recorded and analyzed. The wetting properties were assessed by measuring the receding and tilting angle of hexadecane on these surfaces. We observed that an improvement of the mechanical robustness was accompanied with a decrease of the liquid repellency.

CPP 46.6 Wed 10:00 Poster A

**Quantification of spontaneous imbibition processes in nanoporous systems** — •Christian Thome and Heiko Rieger — Universität des Saarlandes, Saarbrücken, Germany

The study of spontaneous imbibition processes in micro- and nanopores is important for various applications like oil recovery, water flow through soil or drug design. In porous media with elongated pores one can observe a dynamical broadening of the imbibition front which is caused by the temporal arrest of some menisci. This effect has also been shown by microfluidic studies in y-shaped junctions. Here the arrest time of the meniscus in the bigger channel is proportional to the feeding channel length. In contrast to microfluidic channels nanofluidic devices have a high surface-to-volume ratio. As an example we consider a system where a piece of nano-porous vycor glass is in contact with a water reservoir. Density fluctuations over intermolecular distances can be important in this system. For this reason we investigate the flow beavior of the imbition process of water in nano-porous vycor glass with molecular dynamics simulations using a simple Lennard Jones model fluid. The imbibition speed of the meniscus and the speed of the fluid layer in direct contact to the wall atoms is estimated as a function of the wall/fluid-particle-interaction-strength. Futhermore we consider a nano-pore-junction connecting 3 nano-pores of different radii. After filling the feeding channel, the liquid penetrates the smaller of the two outgoing channels and arrests in the bigger one. The arrest time of the meniscus in the bigger tube is determined as a function of the feeding channel length for different junction geometries.

CPP 46.7 Wed 10:00 Poster A

**What controls the wettability of bidisperse bead pack?** — •Robabeh Moosavi[1], Julie Murison[1], Thomas Hiller[1], Martin Brinkmann[1,2], and Matthias Schröter[1] — [1]Max-Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Universität des Saarlands, Saarbrücken, Germany

We report experiments on liquid two-phase flow in bidisperse bead packs. The bidisperese bead pack consists of small and large beads which are either oil wetting or water wetting. The aim of this work is to understand which property of the prepared sample determines its average wettability and how this is linked to the residual oil saturation. To characterize the different samples we measure the capillary pressure saturation curves (CPSC) where the sample is alternately invaded by water and oil. In addition to the CPSC experiments we also carried out x-ray tomography and numerical simulations of two-phase flow with wetting using multi-particle collision dynamics (MPCD). So far, the comparison of the different methods indicate that segregation of beads in the CPSC experiment may have an effect on the determination of the average wettability of the sample.

CPP 46.8 Wed 10:00 Poster A

**Continuum approach to the statics and dynamics of two-phase systems** — •Nikita Tretyakov[1], Jasna Zelko[1], Kostas Ch. Daoulas[1], and Burkhard Dünweg[1,2,3] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Institute for Solid State Research, TU Darmstadt, Germany — [3]Dept. of Chemical Engineering, Monash University, Australia

The most appropriate theoretical description of, e.g., droplets near surfaces, and similar systems, is computational modeling based upon continuum thermodynamics (statics) and hydrodynamics (dynamics).

In the statical case, we present a field-theoretical description [1, 2] of water-vapor interface in the vicinity of a corrugated substrate at nanoscale. The virtue of the method consists in the possibility to derive and calculate the free energy of the system [3].

In the dynamical case, we propose a fully consistent formulation of the lattice Boltzmann method for two-phase fluids (liquid-vapor coexistence) [4]. To this end, one employs the Chapman-Enskog expansion up to the 3rd order and introduces a correction current to fulfill the continuity equation.

[1] K. M. Hong and J. Noolandi, Macromolecules , 14, 3, 1981.

[2] G. H. Fredrickson, The equilibrium theory of inhomogeneous polymers, Oxford, 2006.

[3] K. Ch. Daoulas and M. Müller, Soft Matter, 9, p. 4097, 2013.

[4] J. Zelko and B. Dünweg, Phys. Rev. E (accepted), arXiv:1402.2920, 2014.

CPP 46.9 Wed 10:00 Poster A

**Modelling surface binding and dissociation of biomolecules** — •Daniel Kappe[1,2], Andreas Hütten[1], and Christian Schröder[2] — [1]1Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Germany — [2]2Bielefeld Institute for Applied Materials Research, University of Applied Sciences Bielefeld, Germany

We performed computer simulations in order to study the binding kinetics of molecules which bind to or dissociate from a finite number of binding sites placed on a sensor surface. We modelled the process using a convection-diffusion equation together with a Robin boundary condition. We compared our results to experimental data obtained by Ritzefeld et al. [1] who studied the binding of PhoB to a functionalized surface by surface plasmon resonance studies. Furthermore, we conducted a parameter sweep which allows us to estimate the rate constants of association and dissociation.

CPP 46.10 Wed 10:00 Poster A

**Cell wall sculpting and microflows in plants and insects.** — •Desislava Todorova[1] and Eleni Katifori[1,2] — [1]Max-Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, USA

Remarkably similar types of corrugated architecture have evolved on the internal surfaces of the organs serving for fluid distribution in vascular plants and insects. We focus on examining the relation between the geometric properties of the xylem vessels of plants and the tracheal cells of insects and their functional adaptation for maximizing water flow and gas delivery and exchange, respectively.

We use computational fluid dynamics techniques to study the low Reynolds number flows which naturally occur in such systems and discuss configurations corresponding to optimal functionality.

CPP 46.11 Wed 10:00 Poster A

**Spontaneous Formation of Nanopatterns in Velocity-**

**Dependent Dip-Coated Organic Films: From Dragonflies to Stripes** — Tomas P. Corrales[1], Mengjun Bai[2], Valeria del Campo[1], Maria Retamal[1], Moshe Deutsch[3], Haskell Taub[2], Klaus Knorr[1], Ulrich G. Volkmann[1], and •Patrick Huber[1,4] — [1]Fac. de Fisica, Pont. U. Santiago, 7820436 (Chile) — [2]Physics and Astronomy Dep., U. of Missouri, Columbia, Missouri 65211 (USA) — [3]Physics Dep., Bar-Ilan U., Ramat-Gan 52900 (Israel) — [4]Materials Physics, Hamburg U. of Technology, D-21073 Hamburg (Germany)

We present a study of thin, n-alkane films on the native oxide layer of a silicon surface, prepared by dip-coating in a n-$C_{32}H_{66}$/n-heptane solution. Electron micrographs reveal two distinct adsorption morphologies depending on the substrate withdrawal speed $v$. For small $v$, dragonfly-shaped molecular islands are observed. For a large $v$, stripes parallel to the withdrawal direction are observed. These have a few hundred micrometer lengths and a few-micrometer lateral separation. Grazing incidence X-ray diffraction and atomic force microscopy show that both patterns are monolayers of surface-normal-aligned C32 molecules. With increasing $v$, the surface coverage first decreases, then increases for $v > v_{cr} \sim 0.15$ mm/s. The critical $v_{cr}$ marks a transition between the evaporation regime and the entrainment regime. The stripes' strong texture and the well defined separation are due to an 2D crystallization in narrow liquid fingers, which result from a hydrodynamic instability in the dip-coated films, akin to the tears of wine phenomenology, see also T. Corrales et al., ACS Nano 8, 9954 (2014).

CPP 46.12 Wed 10:00 Poster A

**Generation of ultra-stable flows for microfluidic devices** — •Annemarie Lüdecke[1] and Stefan Diez[1,2] — [1]B Cube - Centre for Molecular Bioengineering, TU Dresden, Arnoldstr. 18, 01307 Dresden, Germany — [2]Max Planck Institute for Molecular Cell Biology and Genetics, Pfotenhauerstr. 108, 01307 Dresden, Germany

In the fast growing field of microfluidics, pumps are essential elements. Notably, the most common pumping system, the volume-driven syringe pump, has two major limitations: (1) the amount of fluid that can be displaced is limited to the syringe volume and (2) the steadiness of the flow is limited by a combination of the step width of the pump motor and the syringe diameter.

Alternative pumping systems, not facing these limitations, rely on pressure differences. When driven by gas pressure, usually requiring external pressure sources like a compressor or a gas bottle, or by osmotic pressure, these pumps require extensive instrumentalization and are comparatively expensive.

When driven by gravitational forces, these pumps often lack long-term steadiness of flow rates. As the fluid moves from the inlet towards the outlet, the height difference equilibrates and hence the driving force diminishes. Here, we present a novel, low-instrumentalization and low-cost method for maintaining an ultra-stable gravitation-driven flow over extended periods of time.

CPP 46.13 Wed 10:00 Poster A

**Switchable imbibition in nanoporous gold** — •Yahui Xue[1,2], Juergen Markmann[1], Huiling Duan[2], Joerg Weissmueller[1,3], and Patrick Huber[3] — [1]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, D-21502 Geesthacht, Germany — [2]State Key Laboratory for Turbulence and Complex Systems, Center for Applied Physics and Technology, Peking University, Beijing 100871, China — [3]Institute of Materials Physics and Technology, Hamburg University of Technology, D-21073 Hamburg, Germany

Spontaneous imbibition enables the elegant propelling of nano-flows because of the dominance of capillarity at small length scales. The imbibition kinetics are, however, solely determined by the static host geometry, the capillarity, and the fluidity of the imbibed liquid. This makes active control particularly challenging. Here we show for aqueous electrolyte imbibition in nanoporous gold that the fluid flow can be reversibly switched on and off through electric potential control of the solid-liquid interfacial tension, that is, we can accelerate the imbibition front, stop it, and have it proceed at will. Simultaneous measurements of the mass flux and the electrical current allow us to document simple scaling laws for the imbibition kinetics, and to explore the charge transport in the metallic nanopores. Our findings demonstrate that the high electric conductivity along with the pathways for fluidic/ionic transport render nanoporous gold a versatile, accurately controllable electrocapillary pump and flow sensor for minute amounts of liquids with exceptionally low operating voltages - see also Y. Xue et al., *Nature Comm.* 5, 4237 (2014).

CPP 46.14 Wed 10:00 Poster A

**Thermocapillary Convection in Microfluidic Devices** — •Lorenz Butzhammer and Werner Köhler — Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany

Thermocapillary convection has been investigated experimentally at a liquid-air interface in a PDMS-based microfluidic device. Fluid dynamics in the vicinity of the meniscus, which is located at a T-junction of the 100-$\mu$m-wide channels, is observed using an inverted light microscope. A temperature gradient along the interface is set up through a focused laser beam (532 nm) and an absorbing dye at a low concentration. This leads to tangential Marangoni stresses and liquid flow towards regions with lower surface tension. Samples included water, ethanol, glycerol and binary mixtures of those with polystyrene beads ($d = 100$-$600\,$nm) for flow visualization. Data evaluation was done using Particle Image Velocimetry (PIV) and Ghost Particle Velocimetry (GPV). Experiments show that the effect is absent in water and water-glycerol mixtures within the investigated temperature range. However, in ethanol, asymmetric convection rolls perpendicular to gravity already arise without an external heat source. The flow strength and direction can be manipulated by laser heating, leading to fluid motion towards lower temperatures. In symmetric mixtures containing ethanol the direction is reversed. Moreover, the onset and strength of the self-induced convection rolls at these concentrations strongly depend on repositioning of the meniscus.

CPP 46.15 Wed 10:00 Poster A

**Equilibration of liquid morphologies in granulates with various wettability** — •Marc Schaber[1], Mario Scheel[3], Martin Brinkmann[2], and Ralf Seemann[1,2] — [1]Experimental Physics, Saarland University, D-66041 Saarbrücken — [2]MPI for Dynamics and Self-Organization, Am Faßberg 17, D-37073 Göttingen — [3]European Synchrotron Radiation Facility, 6 rue Jules Horowitz, F-38000 Grenoble

When adding liquid to dry granulates, the liquid forms a network of capillary bridges and more complex liquid structures. Depending on wettability of the granules and geometry of the granular pile different liquid structures are formed. By means of ultrafast X-ray microtomography we explore the liquid equilibrium distribution emerging within granular packs. Monodisperse glass and basalt microspheres of different diameters are used as granules having small and large contact angle, respectively. By fluidizing the granulate, the packing geometry of the granules is changed and the liquid equilibrium structures are destroyed. We explore time resolved how the liquid is re-distributed and how the liquid morphologies are re-formed into a new equilibrium situation. We find a correlation between the bead diameter and the viscosity of the added liquid to the characteristic equilibration time. The absence of the equilibrium process for non-wettable beads indicates that the liquid redistribution proceeds via a thin liquid wetting film on the surface of the beads.

CPP 46.16 Wed 10:00 Poster A

**Droplet morphologies upon volume change on structured substrates** — •Carsten Herrmann[1], Ciro Semprebon[2], Martin Brinkmann[1,2], and Ralf Seemann[1,2] — [1]Experimental Physics, Saarland University, 66041 Saarbrücken — [2]Max 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 groove geometries with triangular, rectangular and sinusoidal 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 46.17 Wed 10:00 Poster A

**Application of rapid prototyping techniques to create microfluidic devices** — •Fabian Schmid-Michels and Andreas Hütten — Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Germany

Microfluidic devices have applications as analytical systems or biomedical devices and are tools to study various (bio-)chemical reactions. Conventional methods for fabrication are etching glass or silicon, or soft lithography to create a mold for poly(dimethylsiloxane) (PDMS).

Soft lithography needs several costly devices and chemicals. By replacing this process with 3D-printing methods like fused filament fabrication, the creation of the mold requires no more chemicals. By using bio-compatible materials it is also possible to directly print simple microfluidic channels for bio-applications. Print resolution below 0.3mm is difficult to achieve and needs careful tuning of the printer. Several techniques and materials are evaluated to achieve better print resolution.

CPP 46.18 Wed 10:00 Poster A

**Force response of actively deformed polymer microdroplets: dependence on the solid/liquid boundary condition** — •Jonas Heppe[1,2], Joshua D. McGraw[2], Roland Bennewitz[1], and Karin Jacobs[1,2] — [1]INM - Leibniz Institute for New Materials, D-66123, Saarbrücken, Germany — [2]Saarland University, Experimental Physics, D-66041, Saarbrücken, Germany

In fluid dynamics, the solid/liquid boundary condition can play a major role in the flow behavior of a liquid. For example, in the dewetting of identical polymer films on weak slip or strong slip substrates, large qualitative and quantitative differences are observed. Therefore, when applying an external load to a liquid resting on such substrates, the measured reaction forces and the ensuing flow should also depend on the boundary condition. We present atomic force microscopy measurements in which the reaction force of a cantilever is measured as the tip pierces liquid polymer micron sized droplets and films. These indentations are done on substrates with tuned slip. Accessing the size, depth and rate dependence of the resulting force distance curves, we show an influence of the slip condition on the dissipated energy and adhesion.

CPP 46.19 Wed 10:00 Poster A

**Pickering-emulsion for catalytic reactions** — •Dmitrij Stehl[1], Adrian Carl[1], Kornelia Gawlitza[1], Regine von Klitzing[1], Tina Skale[2], Anja Drews[2], Lena Hohl[3] und Matthias Kraume[3] — [1]Physikalische Chemie, TU Berlin, Straße des 17. Juni 124, 10623 Berlin — [2]Verfahrenstechnik in Life Sci. Eng., FB 2, HTW Berlin, Wilhelminenhofstr. 75 A, 12459 Berlin — [3]Verfahrenstechnik, TU Berlin, Frauenhoferstr. 33-36, 10587 Berlin

A Pickering-emulsion (PE) was reported by RAMSDEN in 1903 for the first time. S. U. PICKERING studied this type of solids-stabilized emulsions systematically. PEs can be used in medicine for drug delivery or for catalytic reactions, for example for the hydroformylation of long chained olefins (1-Dodecene) in a water in oil (w/o-) emulsion. In this study, the water droplets (water phase) which are surrounded by SiO2-nanoparticles as stabilizer, contain [HRh(CO)(TPPTS)3] (TPPTS = 3,3',3"-Phosphanetriyltris (benzenesulfonic acid) trisodium salt) as homogeneous catalyst. The solids-stabilized water droplets are emulsified in 1-Dodecene (oil phase). After the hydroformylation, the water droplets with the catalyst can be easily separated from the product by membrane filtration and used again for the next reactions. Preliminary experiments showed that an increase in amount of SiO2-nanoparticles led to an augmentation of the product yield (Tridecanal) and decrease the droplet size from 0,02 to 0,005 mm. An addition of surfactant (Triton X-100) at low concentration (< cmc) increases the product yield as well but has no effect on the droplet size, which is surprising.

CPP 46.20 Wed 10:00 Poster A

**Inertial migration of elastic capsules in Poiseuille flow** — •Kevin Irmer, Christopher Prohm, and Holger Stark — Institute of Theoretical Physics, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

The influence of inertia on the rheology of deformable particles such as capsules, vesicles and red blood cells in flow has attracted much interest over the last few years. Many applications in biology and medical sciences rely on inertial effects. Especially the separation of particles like cancer cells from red blood cells plays an important role.

Using Lattice-Boltzmann simulations, we study the dynamics of a single deformable capsule in microfluidic channels with rectangular cross sections for intermediate Reynolds numbers.

In the channel cross section the capsules migrate towards stable equilibrium positions. We find that the locations of these positions shift towards the channel center for increasing deformability of the capsule and decreasing inertia of the flow. In particular, they strongly depend on deformability quantified by the capillary number. Hence we present a new possibility to separate capsules and other deformable particles by size and deformability. For Reynolds numbers below 100, the equilibrium positions collapse onto a single master curve depending only on the Laplace number.

Finally we determine lift force profiles for channel cross sections with different aspect ratios. The profiles determine inertial migration in the cross section.

## CPP 47: P12: Glasses and Glass Transition

Time: Wednesday 10:00–13:00 Location: Poster A

CPP 47.1 Wed 10:00 Poster A

**The effect of finite temperatures on jammed packings** — •Clemens Buss[1], Claus Heussinger[2], and Oskar Hallatschek[3] — [1]Max-Planck-Institut für Dynamik und Selbstorganisation (MPIDS) Bunsenstrasse 10, D-37073 Göttingen — [2]Institute for theoretical Physics University of Goettingen Friedrich Hund Platz 1 37077 Goettingen — [3]Department of Physics University of California 366 LeConte Hall MC 7300 Berkeley, CA, 94720-7300

We study the effect of finite temperatures on jammed packings. The packings are obtained through a standard energy minimization protocol. We then study their thermodynamic properties by simulating them at finite temperature through a Monte Carlo Metropolis scheme. Based on our simulation model, we can determine mechanical and thermodynamical properties and how they behave for different temperatures, external pressure and coordination numbers. The quantities we measure comprise the thermal expansion, bulk and shear modulus as well as the phase diagram. Together with theoretical arguments we can explain crucial parts of the results and the scaling behaviour. In the last step we connect those findings to real materials such as silica glass.

CPP 47.2 Wed 10:00 Poster A

**Molecular dynamics of polymethylphenylsiloxane under 1-D and 2-D geometrical confinement- a comparison** — •Wycliffe K. Kipnusu[1], Mohamed Elsayed[2], Emmanuel U. Mapesa[1], Reinhard Krause-Rehberg[2], and Friedrich Kremer[1] — [1]Institute of Experimental physics I, Linnstr.5, 04103, Leipzig — [2]Martin-Luther-Universität Halle-Wittenberg)

Molecular dynamics of polymethylphenylsiloxane (PMPS) in 1-D (thin films) and 2-D (silica nanopores with pores sizes of 8, 6, and 4 nm) geometrical constraints are studied by broadband dielectric spectroscopy (BDS) while Positron annihilation lifetime spectroscopy (PALS) is employed to probe the free volume in the bulk PMPS and under 2D confinement. The glass transition temperature (Tg) of thin films down to 5 nm remained bulk-like but the Tg decreases with the reduction of pores sizes for 2-D confinement where additional interfacial relaxation process is observed. This process is removed after silanization of the pores. The change in Tg is attributed to the reduction of density of bulk-like molecules at the center of the pores. This is proven by the PALS results which indicate that the average free volume increases with decreasing pore sizes. This shows how the dimensionality of confinement and packing density of the molecules impacts on the molecular dynamics.

CPP 47.3 Wed 10:00 Poster A

**Glass transition coopeativity from broad band heat capacity spectroscopy** — •Yeong Zen Chua[1], Gunnar Schulz[1], Evgeni Shoifet[1], Heiko Huth[1], Reiner Zorn[2], Jürn W.P. Schmelzer[1], and Christoph Schick[1] — [1]Institute of Physics, University of Rostock, Wismarsche Str. 43-45, 18051 Rostock, Germany — [2]Juelich Centre for Neutron Science, 52425, Juelich, Germany

Molecular dynamics is often studied by broad band dielectric spectroscopy (BDS) because of the wide dynamic range available and the large number of processes resulting in electrical dipole fluctuation and with that in a dielectrically detectable relaxation process. Calorimetry on the other hand is an effective analytical tool to characterize phase and glass transitions by its signatures in heat capacity. In the linear response scheme, heat capacity is considered as entropy compliance. Consequently, only processes significantly contributing to entropy fluctuations appear in calorimetric curves. The glass relaxation is prominent example for such a process. Here we present complex heat capacity at the dynamic glass transition (segmental relaxation) of polystyrene (PS) and poly(methyl methacrylate) (PMMA) in a dynamic range of 11 orders of magnitude, which is comparable to BDS. As one of the results, we determine the temperature dependence of the characteristic length of the corresponding fluctuations. The characteristic length decreases from about 4 nm to about 0.7 nm in the temperature range from 370 K to 500 K. This proves an estimate for possible confinement effects on the segmental relaxation, which is different from vitrification as discussed by Cangialosi et al.

CPP 47.4 Wed 10:00 Poster A

**Glass transition coopeativity from broad band heat capacity spectroscopy** — •Yeong Zen Chua[1], Gunnar Schulz[1], Evgeni Shoifet[1], Heiko Huth[1], Reiner Zorn[2], Jürn W.P. Schmelzer[1], and Christoph Schick[1] — [1]Institute of Physics, University of Rostock, Wismarsche Str. 43-45, 18051 Rostock, Germany — [2]Juelich Centre for Neutron Science, 52425, Juelich, Germany

Molecular dynamics is often studied by broad band dielectric spectroscopy (BDS) because of the wide dynamic range available and the large number of processes resulting in electrical dipole fluctuation and with that in a dielectrically detectable relaxation process. Calorimetry on the other hand is an effective analytical tool to characterize phase and glass transitions by its signatures in heat capacity. In the linear response scheme, heat capacity is considered as entropy compliance. Consequently, only processes significantly contributing to entropy fluctuations appear in calorimetric curves. The glass relaxation is prominent example for such a process. Here we present complex heat capacity at the dynamic glass transition (segmental relaxation) of polystyrene (PS) and poly(methyl methacrylate) (PMMA) in a dynamic range of 11 orders of magnitude, which is comparable to BDS. As one of the results, we determine the temperature dependence of the characteristic length of the corresponding fluctuations. The characteristic length decreases from about 4 nm to about 0.7 nm in the temperature range from 370 K to 500 K. This proves an estimate for possible confinement effects on the segmental relaxation, which is different from vitrification as discussed by Cangialosi et al.

## CPP 48: P13: Charged Soft Matter

Time: Wednesday 10:00–13:00 Location: Poster A

CPP 48.1 Wed 10:00 Poster A

**Dynamics of the Hydrogen Bond Network of Water** — •Miriam Jahn and Stephan Gekle — University of Bayreuth, Germany

The special properties of liquid water originate from the presence of hydrogen bonds that link the molecules in a preferably tetrahedral arrangement. An evidence of the resulting real network structure is the occurrence of loops of hydrogen bonds. Six and seven-membered loops appear most frequently. As the binding energy amounts to few $k_BT$ this network is highly transient.

Using molecular dynamics simulations of bulk water we analyze the dynamics of the network. Based on the assumption that every hydrogen bond is subject to the same molecular rearrangement processes, loops are expected to be more fragile the more hydrogen bonds they contain. This tendency proves to be true except for three and four-membered loops which are unexpectedly short-lived. We find that loops of five, six or seven molecules experience some stabilization that leads to a longer lifespan than indicated by the same number of randomly grouped hydrogen bonds.

CPP 48.2 Wed 10:00 Poster A

**Shape and Stability comparison of various Nanocellulose Crystals** — •Uhlig Martin[1], Andreas Fall[2], Gustav Nyström[2], Maren Lehmann[1], Sylvain Prèvost[1], Lars Wargberg[2], and Regine von Klitzing[1] — [1]Department of Chemistry, TU Berlin, Berlin, Germany — [2]Department of Fiber and Polymer Technology, KTH Royal Institute of Technology, Stockholm, Sweden

Nanocellulose Crystals (NCC) extracted from native cellulose are a promising natural material. Due to their high stiffness, high aspect ratio, water solubility and low cost they are interesting for a lot of applications e.g. in nanocomposites. The most used NCC is sulfuric acid hydrolyzed NCC. Modifying the NCC, e.g. by carboxylation or coating with polyethylene glycol amine (PEG-NH2) overcomes the problem of aggregation. This contribution focuses on the characterization of modified NCCs using Small Angle Neutron Scattering (SANS), Dynamic Light Scattering (DLS) and Transmission Electron Spectroscopy (TEM). DLS is used to investigate the increase in stability of modified NCC compared to unmodified one. SANS and TEM are used to investigate the change in shape and structure of modified NCC. Uncoated NCC both with sulfate groups and carboxylic groups were analyzed. Polymer coated NCC were prepared, either by electrostatic adsorption of polyethyleneimine (PEI) or chemically grafting of polyethylene glycol amine (PEG-NH2) to the NCC particles surface. Aqueous NCC dispersions where measured at various NCC and polymer concentrations and different polymer molecular weights. SANS data revealed a tendency of the rods to aggregate into 2D-stacks of several rods.

CPP 48.3 Wed 10:00 Poster A

**Developing simultaneous actuating and self-sensing technique for IPMC** — •parisa bakhtiarpour, othmar marti, and masoud amirkhani — Institute of experimental physics, Ulm university, Germany

Electroactive polymer (EAP) is a class of material, which deforms under electrical stimulation. Ionic polymer metal composite (IPMC) is a type that can function in the both wet and dry mediums. IPMC is a perfluorinated sulfonic ionic polymer membrane sandwiched between two metallic electrodes and containing mobile cations and fixed anion. Application of IPMC as a smart material in soft robotic is an emerging and cutting-edge technology with a great potential to benefit aerospace, medical and automotive industry. However, a smart system requires a self-sensing mechanism, which allows interacting with environment and responding correspondingly. In this poster, we present a new simultaneous actuating and sensing technique, which is based on the resistance properties of IMPC across the sample.

CPP 48.4 Wed 10:00 Poster A

**The effect of miniaturization on the performance of IPMC** — •virendra vikram singh, parisa bakhtiarpour, othmar marti, and masoud amirkhani — Institute of experimental physics, Ulm university, Germany

Ionic Polymer Metal composites (IPMC) are electroactive polymer (EAP) that bends in response to a small applied electric field as a result of the mobility of cations in the polymer network. IPMC is made of an Ionic polymer membrane such as Nafion covered on both sides by metallic layers, to form the electrodes. This type of polymer is light material and needs a low driving voltage so it is an excellent candidate for smart microelectromechanical systems (MEMS). However, using IPMC for smart MEMS is still a cutting-edge technology, and many modifications and improvements must be done for real-world applications. As a first step, one should understand the performance of IPMC in the millimeter and micrometer scale. Generally, IPMC thickness is around 0.2 mm but length and width are several orders of magnitude bigger than the thickness. Here we present results of actuating and sensing ability when the width and thickness of IPMC are in the same order of magnitude.

CPP 48.5 Wed 10:00 Poster A

**The charge storage properties and applications of polymer brush electret** — •Xinlei Ma — Research Center for Bioengineering and Sensing Technology, University of Science & Technology Beijing, Beijing 100083, People's Republic of China.

Electrets are dielectric materials that can store electrostatic charge over a long time scale. Although benefitting from the charge storage, such materials are widely used in electronics, machinery and biological systems. , challenges remain in principles explanation, facial processing and applications. The polyelectrolyte brush, which anchoring to a substrate with one end of the polymer chain and maintaining lots of fixed ions and counter ions on the surface will bring a further scope on the charge storage mechanism of polymer electrets. Of note, the polyelectrolyte brushes exhibit excellent environment robustness and well-organized chain conformation. Those properties endow superior control over surface structures and functionalities such as film morphology, grafting density, chemical composition, and many other surface properties, which will provide a feasible means to complicated structure fabrication and flexible sensor architecture.

CPP 48.6 Wed 10:00 Poster A

**Simulation of ionic solutions with the extended ReaxFF+ force field** — Oliver Böhm, •Stephan Pfadenhauer, and Philipp Plänitz — AQcomputare GmbH, 09125 Chemnitz, Germany

The ReaxFF+ [1] force field is an extension of the original bond order dependend reactive force field (ReaxFF) of the van Duin group [2]. The capability of the ReaxFF+ force field to simulate ionic solutions is demonstrated on the example of hydrolysis of sodium clusters. The large number of parameters were fitted to DFT ab initio data by means of an improved training algorithm. The predictions of the ReaxFF+ simulations are in good agreement with ab inito results. Therefor we have shown that ReaxFF+ is capable of describing covalent as well as ionic bonds.

[1] O. Böhm, et al., J. Am. Chem. Soc. (2015) submitted

[2] A. van Duin, et al., J. Phys. Chem. A, 105, 9396 (2001); J. Phys. Chem. A, 107, 3803 (2003)

CPP 48.7 Wed 10:00 Poster A

**Quasi-elastic neutron scattering study of a room temperature ionic liquid confined in nanoporous carbon** — •Mark Busch[1], Jan Embs[2], Boris Dyatkin[4], Katie Van Aken[4], Alexei Kornyshev[3], Yury Gogotsi[4], and Patrick Huber[1] — [1]Institut für Werkstoffphysik und Werkstofftechnologie, TU Hamburg-Harburg, Hamburg, Deutschland — [2]Laboratory for Neutron Scattering, Paul Scherrer Institut, Villigen, Schweiz — [3]Imperial College, London, UK — [4]Drexel University, Philadelphia, U. S. A.

We present quasi-elastic neutron scattering measurements of the self-diffusion behaviour of the room temperature ionic liquid 1-N-butylpyridinium bis-((trifluoromethyl)sulfonyl)imide which was confined in nanoporous carbon. Thereby the influence of different pore diameters in the nanometre range on the self-diffusion dynamics has been investigated at several temperatures.

CPP 48.8 Wed 10:00 Poster A

**Solvation of model spheres in different ionic liquids** — •Volker Lesch[1], Andreas Heuer[1], Christian Holm[2], and Jens Smiatek[2] — [1]Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster — [2]Institut für Computerphysik, Universität Stuttgart

Due to their ionic properties ionic liquids are considered to be solvents for the future. Furthermore, their toxic level is low compared with other solvents. However, in the literature only the solvation of cellulose and zinc finger is investigated via molecular dynamics but no general discussion of solvation effects is available.

In this study, we focus on the solvation of charged and uncharged model spheres in 1-ethyl-3-methylimidazolium (emim) with the anions chloride, tetrafluoroborate, acetate and bis(trifluoromethanesulfonyl)imide. Beside the investigation of different anions, we also simulate the model spheres with different $\epsilon$ values. We found a dramatic influence of the anion size on the structuring of the ionic liquid, especially for the charged spheres.

## CPP 49: P14: Polymer Dynamics

Time: Wednesday 10:00–13:00 Location: Poster A

CPP 49.1 Wed 10:00 Poster A

**Molecular dynamics and charge transport in polyisobutylene-based ionic liquids** — •Falk Frenzel[1], Makafui Yao Folikumah[2], Matthias Schulz[2], Wolfgang Binder[2], and Friedrich Kremer[1] — [1]Institute of Experimental Physics I, University of Leipzig, Linnéstr. 5, 04103 Leipzig, Germany — [2]Institute of Chemistry, Martin-Luther-University Halle-Wittenberg, Von-Danckelmann-Platz 4, 06120 Halle (Saale), Germany

Broadband dielectric spectroscopy (BDS) and differential scanning calorimetry (DSC) are employed to study molecular dynamics and charge transport in polyisobutylene(PIB)-based ionic liquids. The latter form a homologous series of polymeric 'Ionic Liquids' containing monovalent and bivalent telechelic PIBs either with N,N,N-triethylammonium as the functional group or 1-methylpyrrilidinium. Three well separated dielectric relaxation processes and a conductivity contribution are obtained. This offers to unravel the interplay between molecular dynamics and charge transport in this novel class of materials.

CPP 49.2 Wed 10:00 Poster A

**Proton Motion in Phosphoric Doped PBI Membranes for HT-PEFC** — •Bernhard Hopfenmüller[1], Reiner Zorn[2], Oxana Ivanova[1], Olaf Holderer[1], Wiebke Maier[3], Werner Lehnert[3], Michaela Zamponi[1], Niina Jalarvo[4], Georg Ehlers[5], and Michael Monkenbusch[2] — [1]JCNS Outstation at MLZ, Forschungszentrum Jülich GmbH, Garching, Germany — [2]JCNS-1 & ICS-1, Forschungszentrum Jülich GmbH, Jülich, Germany — [3]IEK-3, Forschungszentrum Jülich GmbH, Jülich, Germany — [4]JCNS-SNS, Forschungszentrum Jülich GmbH, Oak Ridge, USA — [5]SNS, Oak Ridge National Laboratory, Oak Ridge, USA

PBI (poly(2,2*-(m-phenylene)-5,5*-bibenzimidazole) membranes with phosphoric acid impregnation are a promising material for high-temperature polymer electrolytemembrane fuel cells (PEMFC). Such membranes tolerate impurities like 1-2% of carbon monoxide produced during operation in PEMFC Systems, show good chemical resistance and high glass transition temperature (about 700*K).The macroscopic level of such materials is well studied but one still lacks a detailed description of the microscopic dynamics, mainly the diffusion of protons. An excellent technique to study such processes is given by Neutron Scattering.We combined Time-Of-Flight and Backscattering to investigate the temperature and q-dependency of proton-diffusion in the membrane materials.

CPP 49.3 Wed 10:00 Poster A

**Dielectric spectroscopy and DSC on water / PEG mixtures** — •Alexander Matt, Björn Kuttich, and Bernd Stühn — Experimental Condensed Matter Physics, TU Darmstadt, Germany

The interplay between water and protein dynamics is an important feature for the functionality of proteins in the human body. The dynamics of polymers in an aqueous environment are a simplified model system for this complex biological situation. Taking a simply structured water soluble polymer instead of a complex protein allows to distinguish between the contributions of the different components to the overall dynamics of the mixture. A well suited method for the investigation of polymer dynamics is dielectric spectroscopy. Measuring in the high frequency range between 200 MHz and 50 GHz both pure water dynamics and also fast polymer dynamics can be investigated as well as their interplay.

In this work we focus on the polymer poly(ethylene glycol) (PEG). Despite its simple structure it shows quite surprising features when dissolved in water, like its hydrophilicity itself for instance. Further more, we find that already low polymer concentrations lead to a complete change in the water dynamics measured by dielectric spectroscopy, indicating a long range disturbance of the hydrogen bonding network. These effects are investigated for a broad range of molecular weights, concentrations and temperatures in order to vary systematically monomer and end-group concentration as well as solubility properties. All dielectric investigations are accompanied by calorimetric measurements.

CPP 49.4 Wed 10:00 Poster A

**Examination of medium-ranged interactions through optical tweezing of a droplet in a multiphase ternary mixture (PNIPAM/H2O/DMSO)** — •Michael Orlishausen and Werner Köhler — Physikalisches Institut, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth

Poly-N-isopropylacrylamide (PNIPAM) in acqueous solution can show a cononsolvency effect when mixed with another solvent. A proper concentration of that solvent can result in the shift from a lower (LCST) to an upper critical solution temperature (UCST). In our case, we chose Dimethylsulfoxid (DMSO) and investigated the resulting ternary system at room temperature, and thus below its UCST, using a light microscope and a laser beam (532 nm) focused through the objective, which was utilized both for optical tweezing and local heating. In an unperturbated state the ternary system the sytem consists of myriads of droplets in different phase states with diameters of several microns. Due to the high refractive index of DMSO as a pure component, DMSO-rich droplets can be easily tweezed. When a tweezed droplet is forced through the sample by controlling the position of the beam, a correlated network-like response of the interacting droplets near the perturbation occurs on a length scale of at least 10 microns. The motion of such a droplet also leads to a net growth of its size as a result of a more frequent contact with other droplets of similar composition, even when only moving on a circular path near the initial position. When a water soluble absorbing dye is added, the temperature field induced by the laser moves along with the tweezed droplet.

CPP 49.5 Wed 10:00 Poster A

**Diffusion of crystalline lamella in a semicrystalline polymer** — •Martin Neumann, Stefan Krause, Christian von Borczyskowski, and Robert Magerle — Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Chemnitz, Germany

During crystallization, elastomeric polypropylene (ePP) with 15 % crystallinity forms isolated $\sim$ 50-nm small crystalline lamella within the amorphous matrix and larger but immobile complexes of crystalline lamella. With Atomic Force Microscopy (AFM) we measured the diffusion of these small lamella in 60 nm thin polymer films at different temperatures and analyzed the diffusion trajectories to extract the diffusion coefficients. The temperature dependence of the data is well described by the Stokes-Einstein-Equation (SEE) and the Williams-Landel-Ferry-Equation (WLF). The size variation of the diffusing crystals led to a broad distribution of diffusion coefficients, which cannot completely be explained by the Stokes-Einstein-Equation (SEE). We identified heterogeneities of the crystal diffusion depending on the distance $d_C$ between isolated crystals and the larger crystalline lamella. Isolated crystals moved up to 5 times slower when $d_C$ was smaller than 50 nm. Our interpretation of this result is that there is an amorphous interphase layer around all crystalline lamella, which has an increased viscosity. This could be due to partly crystallized polymer coils, which are not able to diffuse like the completely amorphous ones.

CPP 49.6 Wed 10:00 Poster A

**Comparison between thermal diffusion of a linear-chain polymer and a polymer microgel** — •Bastian Pur[1], Werner Köhler[1], Klaus Huber[2], and Martin Schneider[2] — [1]Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Physikalische Chemie, Universität Paderborn, 33098 Paderborn, Germany

In present theories for polymer thermophoresis in dilute solutions there are two theoretical models under discussion: draining coil and nondraining coil, corresponding to the Rouse and the Zimm picture, respectively. In order to discriminate between these models we have started a comparative investigation of a linear-chain polymer and a cross-linked microgel. The linear polymer sample used is poly(methylmethacrylate) (PMMA) and the microgel sample is PMMA, crosslinked with ethylene-glycol-dimethacrylate (EGMA). In either case toluene is used as solvent. By means of transient holographic grating technique we obtained the thermal diffusion coefficient $D_T$, the Fickian diffusion coefficient $D$ and the Soret coefficient $S_T$ as functions of the polymer concentration $c$. We have found that for $c \to 0$ the thermophoretic mobility of the linear polymer and the microgel are identical within experimental accuracy. The PMMA microgel shows, however, a significantly faster decay with increasing concentration, which we interprete as a result of the more rapidly increase of the microscopic friction.

# CPP 50: P15: Polymers and Fields

Time: Wednesday 10:00–13:00 Location: Poster A

CPP 50.1 Wed 10:00 Poster A

**Molecular structure of azobenzene-containing systems from classical MD simulations** — •Olga Guskova[1], Vladimir Toshchevikov[1], Jaroslav Ilnytskyi[1,2], and Marina Saphiannikova[1] — [1]Leibniz-Institut für Polymerforschung Dresden e. V., Theorie der Polymere, Hohe Str. 6, 01069 Dresden, Deutschland — [2]National Academy of Sciences of Ukraine, Institute for Condensed Matter Physics, Svientsitskii Str. 1, 79011 Lviv, Ukraine

Azobenzene-containing side chain polymers [1,2] and molecular glasses based on propeller-like C3-symmetric azobenzene mesogenes [3] are investigated in classical molecular dynamics simulations. Two length scales are considered: (i) the molecular level with atomistic resolution, where reversible conformational changes of azobenzene chromophores upon light illumination lead to contractions/extensions of low amplitudes due to a limited size of mesogene groups, and (ii) the mesoscopic level, where light-induced molecular movements are observed over larger distances, comparable with the gyration radius of polymer chains. The influence of isomerization and orientation mechanisms on molecular structure and light-induced deformation is elucidated.

[1] J. Ilnytskyi et al., J. Chem. Phys. 135, 044901 (2011).

[2] M Saphiannikova et al., Proceedings of SPIE "Optical Materials and Biomaterials in Security and Defence Systems Technology X", 8901, 890138 (2013).

[3] N.S. Jadavalli et al., Appl. Phys. Lett. 105, 051601 (2014).

CPP 50.2 Wed 10:00 Poster A

**An alternative theoretical description of magneto-sensitive elastomers** — •Dirk Romeis and Marina Saphiannikova — Leibniz-Institut für Polymerforschung Dresden e.V.

Magnetorheological elastomers are composites that consist of magnetically permeable particles incorporated into an elastic (polymer) matrix. As a magnetic field is applied to such material a deformation and changes in the mechanical properties take place. In experiments often a stretching of the sample in direction parallel to the external field is reported. In contrast, many theoretical approaches to describe such systems predict a compression in the field direction. We present an alternative microscopic approach for magneto-sensitive elastomers in an external magnetic field and find a behavior in agreement with the experimental observation. For any parameter set our results always predict a stretching in direction of the field.

CPP 50.3 Wed 10:00 Poster A

**Multifunctional Magnetic Hydrogel Particles** — •Marcus Witt, Sebastian Backes, and Regine von Klitzing — Technische Universität Berlin, Physikalische Chemie, Germany

Microgels made of N-isopropylacrylamide (NIPAM) exhibit a volume phase transition temperature (VPTT) which leads to reversible swelling in water. The swelling and shrinking depends on the temperature, and with addition of different co-monomers also on the pH and ionic strength.

With the incubation of magnetic nanoparticles (MNP) such as cobalt ferrite we can obtain ferrogels which are also responsive to external magnetic fields.

Most publications about ferrogels are based on core/shell particles. In contrast, we aim for a homogenous distribution of MNP over the whole hydrogel, so that the ferrogel should respond uniformly to the applied magnetic field. Therefore, we synthesized a homogenously crosslinked hydrogel by a constant feeding of the reactant. The MNP are then incubated by mixing aqueous solutions of hydrogel and MNP.

We were able to show that the initial thermoresponsive properties of the hydrogel are preserved for ferrogels both in bulk solution and adsorbed on a Si-surface.

Measurements of adsorbed ferrogel particles in an external magnetic field parallel to the surface have been carried out by AFM. First results show an increase of particle height and volume with an increasing magnetic field, whereas the area of the particle changes only slightly.

CPP 50.4 Wed 10:00 Poster A

**In situ polymerization of organic conductive thin films** — •Jenny Lebert and Eva M. Herzig — TU München, Munich School of Engineering, Lichtenbergstr. 4, 85748 Garching

Organic semiconducting materials can be applied in optoelectronic devices such as organic light-emitting diodes and organic solar cells.

The conductivity and optoelectronic properties of polymers strongly depend on their molecular morphology and crystallization behavior. Therefore controlling the thin film morphology is one of the main challenges when it comes to developing fabrication processes that work in small labs as well as in large industrial scales. Moreover, a profitable scale-up requires the use of low-priced and available materials.

In situ polymerization of the active material is a promising approach for the fabrication of conductive thin films, as it combines the use of cheap materials with the possibility to control the film morphology. In this work, different synthetic chemical routines are combined with systematic physical analyses to investigate varying systems. The obtained polymer films are analyzed regarding their optic and optoelectronic properties, their conductivity and morphology. Additionally they are employed as active layers in organic solar cells.

CPP 50.5 Wed 10:00 Poster A

**A FM-SFM study of the self-assembly of organic molecules on Au(111)** — •Sebastian Schneider, Kushtrim Bytyqi, Michael Marz, Carmen Pérez León, and Regina Hoffmann-Vogel — Karlsruher Institut für Technologie, Physikalisches Institut, D-76131 Karlsruhe

Molecular self-assembly at solid interfaces is governed by the delicate balance between competing molecule-substrate and molecule-molecule interactions. Therefore, the substrate temperature during deposition, post-annealing of the sample and the molecular coverage influence the self-assembly process. Noble metal surfaces are widely used as substrates because of their low chemical reactivity. We have investigated 10,10'-dibromo-9,9'-bianthryl (DBBA) on Au(111) with frequency modulation scanning force microscopy. DBBA is well-known as precursor for graphene nanoribbons [1]. Depending on the coverage, different self-assembled molecular structures are observed on the surface. For low coverage, the molecules arrange along the herringbone reconstruction of the Au(111) (HB-phase). With increasing coverage, a new phase of molecular islands appear coexisting with the HB-phase. These islands display a stripe-like structure of highly ordered molecules.
[1]J. Cai, P. Ruffieux, R. Jaafar, M. Bieri, T. Braun, et al., Nature **466**, 470,(2010)

CPP 50.6 Wed 10:00 Poster A

**A scanning force microscopy study of the growth of organic molecules on Au(111)** — •Kushtrim Bytyqi, Sebastian Schneider, Michael Marz, Carmen Pérez León, and Regina Hoffmann-Vogel — Karlsruher Institut für Technologie, Physikalisches Institut, D-76131 Karlsruhe

Recently, J. Cai et al. succeeded in the fabrication of graphene nanoribbons (GNRs) on the crystalline surface of noble metals via on-surface chemical synthesis [1]. They showed that armchair edge GNRs can be grown on Au(111) using 10,10'-dibromo-9,9'-bianthryl (DBBA) as precursor molecules following a three-step process [1,2].
We have investigated the ordering of DBBA molecules on Au(111) by frequency modulation scanning force microscopy at room temperature (RT) in ultrahigh vacuum. The molecules were evaporated on clean Au(111). During deposition, the substrate was either kept at RT and subsequently annealed to $\sim 200^{\circ}$C, or was preheated to $\sim 200^{\circ}$C. The coverage of the molecules was modified by varying the evaporation time. We have observed different molecular configurations depending on the experimental conditions. Among others, we imaged molecular islands with a stripe-like ordering apparently consisting of two distinct phases.

[1] J. Cai et al., Nature **466**, 470 (2010).
[2] van der Lit et al., Nature Commun. **4**, 2013 (2013).

CPP 50.7 Wed 10:00 Poster A

**On-surface polymerization of flexible molecular wires** — Christophe Nacci[1,2], Francisco Ample[3], David Bleger[4], Stefan Hecht[4], Christian Joachim[5], and •Leonhard Grill[1,2] — [1]Fritz-Haber-Institute, Berlin, Germany — [2]Department of Physical Chemistry, University of Graz, Austria — [3]IMRE, Singapore — [4]Department of Chemistry, Humboldt-Universität zu Berlin, Germany — [5]CEMES-CNRS, Toulouse, France

The on-surface polymerization of molecular building blocks on a Au(111) surface is studied by scanning tunneling microscopy and spectroscopy at low temperatures in combination with calculations. While rather rigid molecular chains, such as graphene nanoribbons, have been grown successfully in the last years, flexible molecular wires remain still a challenge. A key issue is here the charge transport capability through the molecule. Chemical linking is achieved by attachment of halogen substituent atoms at specific molecular sites in the ex-situ synthesis. After deposition under ultrahigh vacuum conditions onto the surface, the chemical reaction is induced by sample heating. We show the successful formation of a flexible polymer that contains various sub-units with characteristic properties directly on the surface. The electronic structure of the molecular wire is studied by spatial mapping of individual molecules.

## CPP 51: P16: New Instruments and Methods

Time: Wednesday 10:00–13:00 Location: Poster A

CPP 51.1 Wed 10:00 Poster A

**Theoretical analysis of vibrating microstructures using dynamic scanning electron microscopy (DySEM)** — •Maria Schröter[1], Matthias Holschneider[2], Martin Ritter[3], Christiane Weimann[1], and Heinz Sturm[1,4] — [1]BAM 6.9, Federal Inst. Materials Research, Berlin — [2]Inst. Mathematics, Univ. Potsdam — [3]Electron Microscopy, TU Hamburg-Harburg — [4]Faculty V, TU Berlin

The poster presented shows the development and verification of a theory, with which the results of a newly developed measuring method (DySEM technique) can be described.

Dynamic Scanning Electron Microscopy is used for measuring the vibrational dynamics of a microscale oscillator at flexural and torsional resonance. In addition to the classical secondary electron (SE) signal, the dynamic part of the signal can be obtained using a lock-in amplifier synchronized to the excitation frequency.

The model of imaging generating mechanism relates the experimental images to the spatio-temporal interaction between electron beam and periodically vibrating microstructure. Furthermore, the material properties of the micro-oscillator as well as the contributions of energy loss mechanisms must be considered for imaging, especially for tapping mode microscopy of soft matter.

The analysis of the imaging of oscillating microstructures by means of scanning electron microscopy is thereby achieved in this poster presented as a combination of experiment, theory and simulation (1).

(1) Schröter, Dissertation TU Berlin (2014)

CPP 51.2 Wed 10:00 Poster A

**Force field conversion and comparison** — •Volker Lesch[1], Carlos E. S. Bernardes[2], Jose Nuno Canongia Lopes[2], Marcello Sega[3], Othmar Steinhauser[3], Christian Schröder[3], Luis Miguel Varela Cabo[4], Hadrian Montes[4], Trinidad Mendez-Morales[4], and Andreas Heuer[1] — [1]Westfälische Wilhelms-Universität Münster — [2]Universidade de Lisboa — [3]Universität Wien — [4]University of Santiago de Compostela

Force fields are the core of each molecular dynamics (MD) simulation but each MD-simulation package has its advantages and drawbacks. Therefore, sometimes a conversion of force fields is necessary which is very tedious and error-prone. Here, we present the conversion tool ForConX (force field based on XML structure). ForConX is written in Python and organized in different moduels for each of the following MD packages: Gromacs, Amber, Charmm, DL_POLY.

Several studies focused on the effect of polarization on simulation results. Here, for the first time we compare two optimized force field and elucidate the real gaps between non-polarizable and polarizable MD-simulations. More specifically, we focus on the limits describing structure and dynamics of the optimized non-polarizable force field OPLS-AA and the optimized polarizable force field APPLE&P.

CPP 51.3 Wed 10:00 Poster A

**3D-cross correlated light scattering in combination with small-angle neutron scattering** — •Yvonne Hertle[1], Annegret Günther[1,2], Fangfang Chu[2], Daniel Clemens[2], Matthias

Ballauff[2], and Thomas Hellweg[1] — [1]Universität Bielefeld, PC III, Universitätsstr. 25, 33615 Bielefeld — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, EM-ISFM, Hahn-Meitner-Platz 1, 14109 Berlin

For researchers, particularly from the field of soft condensed matter, scattering techniques are an important element for the characterization of a wide variety of systems. Light scattering (LS) is suitable to determine the overall particle shape and size, however, small-angle neutron scattering (SANS) provides information of the internal structure. The big difference between these two methods is the concentration range in which the samples are characterized. Conventional LS-experiments can only be performed on diluted samples to assure that only single-scattered light is detected, while for a SANS-measurement highly concentrated samples are required. In order to measure highly concentrated samples with LS, a 3D-LS setup is used, where multiple scattering is eliminated by performing two simultaneously light scattering experiments. Currently a combination of 3D-LS with a small-angle neutron scattering instrument (V16) at the Helmholtz-Zentrum in Berlin is build up to measure simultaneously two different scattering experiments on the same sample.

CPP 51.4 Wed 10:00 Poster A

**Glassy dynamics of polymer brushes: employing an equivalent circuit model to analyze broadband dielectric spectroscopy data** — •Martin Tress[1], Nils Neubauer[1], Rene Winkler[2], Petra Uhlmann[2], Emmanuel Urandu Mapesa[1], Manfred Reiche[3], and Friedrich Kremer[1] — [1]University of Leipzig, 04103 Leipzig, Germany — [2]Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany — [3]Max Planck Institute of Microstructure Physics, 06120 Halle (Saale), Germany

The glassy dynamics of poly(2-vinylpyridine) (P2VP) polymer brushes is investigated by means of Broadband Dielectric Spectroscopy (BDS). For that, P2VP brushes are grafted onto an ultra-flat, highly conductive silicon electrode. The latter is part of a recently developed nano-structured electrode arrangement which has been refined to achieve an electrode-to-electrode distance of only ~40 nm. Since the studied brushes exhibit thicknesses between 1.8 to 7 nm, a major fraction of the capacitor volume is empty. To consider the impact of this partial filling as well as the other components in the capacitor (e.g. nano-structure spacers) a sophisticated equivalent circuit model is implemented in the fit function. This enables to unravel polarization effects, charge transport and molecular relaxation.

CPP 51.5 Wed 10:00 Poster A

**Determination of Volatility of Ionic Liquids at the Nanoscale by means of Ultra-Fast Scanning Calorimetry** — •Mathias Ahrenberg[1], Martin Beck[2], Christin Schmidt[3], Sergey P. Verevkin[3], Olaf Kessler[2], Udo Kragl[3], and Christoph Schick[1] — [1]Institut für Physik, Universität Rostock — [2]Maschinenbaufakultät, Universität Rostock — [3]Institut für Chemie, Universität Rostock

Ionic Liquids (ILs) are intend to be used as quenching media in the heat treatment of metallic materials, e.g. aluminum alloys, even the solution annealing temperature of such alloys is 800 K. The most thermally stable ILs exhibit an onset temperature of decomposition at about 620 K as measured with slow scanning methods, e.g. TGA. Since in a real quenching process the IL is exposed to high temperature only shortly and in a thin layer surrounding the alloy gives reason to investigate the IL at such small scales in time and space. Here we present a new method for the determination of the mass loss rate of such liquids using differential fast scanning calorimetry. We have developed and proven this method using [EMIm][NTf2] and [BMIm][NO3] at temperatures of up to 750 K and in different atmospheres to distinguish between decomposition and evaporation. It was demonstrated that evaporation is still the dominating process of mass loss even at such highly elevated temperatures. In addition, since the method allows very high heating rates (up to 10,000,000 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.

## CPP 52: Focus: Electrolytes at Interfaces - Stern Layer (joint session with CPP, BP)

Time: Wednesday 15:00–18:00 Location: C 130

**Invited Talk** CPP 52.1 Wed 15:00 C 130

**Ultraslow dynamics of hydrated metal ions at the water-solid interface observed by atomic force microscopy** — •Kislon Voitchovsky — Durham University, Durham, UK

The lateral organisation and dynamics of ions in the Stern layer of immersed solids is central to many electrochemical and biological processes. However, measuring the lateral organisation and dynamics of single adsorbed ions remains challenging experimentally. Recently we showed that atomic force microscopy could be used to image single metal ions at the surface of various solids in water [1, 2]. Our results indicate that, depending on the hydration landscape of the solid, adsorbed ions can form ordered structures within the Stern layer, through correlation effects that are driven purely by the interfacial water [2]. The dynamics of the adsorbed ions appears surprisingly slow, typically exhibiting residence times above the millisecond. This suggests that water can also dramatically alter the ions dynamics and play a key role in stabilizing adsorbed ions at a given location of the interface. The existence of long-lived ionic structures at interfaces could have important implications for charge transfer and at biointerfaces.

[1] M. Ricci, P. Spijker, F. Stellacci, J.-F. Molinari, K. Voitchovsky, Langmuir, 29, 2207 (2013) [2] M. Ricci, P. Spijker, K. Voitchovsky, Nature Commun., 5, 4400 (2014)

CPP 52.2 Wed 15:30 C 130

**Direct observation of ionic structure at solid-liquid interfaces: A deep look into the Stern Layer** — •Igor Siretanu, Daniel Ebeling, Martin P. Andersson, Cunlu Zhao, Dirk van den Ende, and Frieder Mugele — Physics of Complex Fluids and MESA+ Institute for Nanotechnology, Department of Science and Technology, University of Twente, PO Box 217, 7500 AE Enschede, The Netherlands

The distribution of ions and charge at solid-water interfaces plays an essential role in a wide range of processes in biology, geology and technology. While study of the solid-electrolyte interfaces date back to the early 20th century, a detailed picture of the structure of the electric double layer has remained elusive, largely because of experimental techniques have not allowed direct observation of the behaviour of ions, i.e. with subnanometer resolution. Making use of recent advances in Atomic Force Microscopy with atomic level precision, herein, we reveal the local surface charge and the ordered adsorption of the divalent ions, unlikely monovalent ions, to heterogeneous clay surfaces in contact with aqueous electrolytes. Complemented by density functional theory, the experiments produce a detailed picture of the formation of surface phases by templated adsorption of cations, anions and water, stabilized by hydrogen bonding.

CPP 52.3 Wed 15:45 C 130

**Probing surface chemistries at mineral surfaces in nanometer-confined electrolytes with atomic force microscopy** — •Cunlu Zhao, Daniel Ebeling, Igor Siretanu, Dirk van den Ende, and Frieder Mugele — Physics of Complex Fluids and MESA+ Institute for Nanotechnology, Department of Science and Technology, University of Twente, PO Box 217, 7500 AE Enschede, The Netherlands

We adopt atomic force microscopy (AFM) to investigate the chemistries of mineral surfaces in nanometer-confined electrolyte solutions. Firstly, AFM was used to measure interaction forces between tip and solid surfaces with nanometer separation in ambient electrolytes. Then a charge regulation (CR) boundary was formulated for the Poisson-Boltzmann equation to establish a linkage between the AFM measured force curves and the surface chemistries (e.g., pK values of surface (de)protonation and ion adsorption). Finally, we analyzed force vs. distance curves recorded between a silica tip and heterogeneous silica-gibbsite substrates in aqueous solutions of NaCl and KCl within the framework of CR boundary-complemented Derjaguin-Landau-Verwey-Overbeek (DLVO) theory. By fitting experimental force vs. distance curves down to tip-sample separation of 2nm, we determined for both silica and gibbsite surfaces pK values of surface (de)protonation and ion adsorption. The various pK values determined from our AFM experiments are quite consistent with the macroscopic titration measurements tabulated in the literature. This indicates that AFM could be potentially used as a titration tool, but with an unprecedentedly high resolution.

CPP 52.4 Wed 16:00 C 130

**Ion adsorption-induced wetting transition in oil-water-mineral systems** — •Frieder Mugele, Bijoy Bera, Andrea Cavalli, Igor Siretanu, Armando Maestro, Dirk van den Ende, Michel Duits, and Martien Cohen-Stuart — University of Twente, MESA+ Institute for Nanotechnology, Physics of Complex Fluids, Enschede, The Netherlands

The relative wettability of oil and water on solid surfaces is crucial to many environmental and technological processes including soil contamination/remediation, oil-water separation, and oil recovery. Good wettability of one fluid generally implies strong retention of that fluid in a porous solid matrix and simultaneously easy displacement of the other one. Here, we demonstrate that the contact angle of aqueous solutions of common chloride salts on mica in ambient oil displays a transition from near zero to finite contact angles up to 10° upon replacing monovalent Na+ and K+ cations in the aqueous phase by divalent Ca2+ and Mg2+ at neutral to elevated pH. This wetting transition is driven by electrostatic forces and originates from charge reversal of the mica-water interface upon adsorption of divalent cations. The ion-induced wettability alteration is synergistically enhanced by small amounts of polar molecules, stearic acid, added to the ambient oil, leading to water contact angles up to 70°.

CPP 52.5 Wed 16:15 C 130

**Cardiolipin Monolayers** — •Renko Kensbock, Heiko Ahrens, Andreas Gröning, Thomas Ortmann, and Chrisitane A. Helm — Physik, Uni Greifswald, 17487 Greifswald, Germany

Cardiolipin-cytochrome c binding in the inner mitochondrial membrane is pertinent to apoptotic processes involving positively charged cytochrome c, motivating a characterization of cardiolipin membranes. Cardiolipins are negatively charged lipids with four alkyl chains. Our approach is to analyse cardiolipin monolayers at the water-air interface, using isotherms and Brewster angle microscopy. The calculation of the in-plane electrostatic pressure consists of an electrostatic contribution using Grahame's equation and a chemical part reflected by the law of mass action. A nonmonotonic ionic strength dependence with a maximum at 0.1 M (NaCl, KCl) is observed for the phase transition surface pressure. This finding is in accordance with the calculations predicting the dominance of charge screening by monovalent counterions only for concentrations above 0.1 M. For lower salt content, its increase causes an elevation of the degree of dissociation and thus electrostatic repulsion within the cardiolipin membrane. The results will be reported, showing pH, concentration, temperature influences on the surface potential, and thus the ability to bind cytochrome c.

### 15 min. break

**Invited Talk** CPP 52.6 Wed 16:45 C 130

**Water flow along a solid interface affects the Stern layer** — •Mischa Bonn — Max Planck Institute for polymer research, Mainz, Germany

At the surface or interface of water, the water hydrogen-bonded network is abruptly interrupted, conferring properties on interfacial water different from bulk water. Owing to its importance for disciplines such as electrochemistry, atmospheric chemistry and membrane biophysics, the structure of interfacial water has received much attention.

We elucidate the structure and structural dynamics of interfacial water using ultrafast surface-specific sum-frequency generation (SFG) vibrational spectroscopy. We make use of the fact that the SFG signal depends critically on the interfacial organization of water molecules.

We attempt to bridge continuum models of laminar flow along interfaces, with molecular-level descriptions of the Stern and diffuse layer, which describe the near-surface distribution of ions. For water at two different mineral interfaces, we report a dramatic effect of water flow water along the mineral surface on the organization of water at the interface. Our observations can be explained by considering the coupling between the flow and the dissolution chemistry at the interface. Even for low-soluble quartz at neutral pH, dissolution plays a key role in determining the interfacial water organization through the charge on the surface.

CPP 52.7 Wed 17:15 C 130

**Breaking the Symmetry of Ions at the Air-Water Interface** — •Eva Brandes[1], Peter Karageorgiev[1], Padmanabhan Viswanath[2], and Hubert Motschmann[1] — [1]Institute of Physical and Theoretical Chemistry, University of Regensburg, D-93040 Regensburg, Germany — [2]Centre for Nano and Soft Matter Sciences, Jalahalli, Bangalore 560013, India

The air-water interface is a widely discussed system. Controversial opinions exist especially for the arrangement of dissolved ions close to the interface; while the classical picture predicts depletion, more recent investigations suggest a nonmonotonous concentration profile with an enrichment layer followed by a depletion layer. A sophisticated method to investigate the air-water interface is the IR-vis sum frequency generation (SFG) spectroscopy, because this method is intrinsically surface specific for soft media.

In this contribution we investigated the behavior of octahedral metal complex ions close to the air-water interface. No SFG signal is expected for octahedrons unless there is a reduction in symmetry. This distortion can only take place close to the interface because only there is a non-isotropic environment. We got SFG responses from the octahedrons, revealing that they are close to the interface. Furthermore we measured the surface excess via a surface tension isotherm, which turns out to be negative. The combined measurements suggest a nonmonotonous concentration profile.

CPP 52.8 Wed 17:30 C 130

**Macro- and Microrheology of Heterogeneous Microgel Packings** — Fany Di Lorenzo[1,2] and •Sebastian Seiffert[1,2] — [1]Freie Universität Berlin, Germany — [2]Helmholtz-Zentrum Berlin, Germany

Microgels are soft deformable colloids that can be packed by external compression. Such packing transforms a suspension of loose microgel particles into an arrested state with properties similar to that of a macroscopic gel. We follow this idea and prepare microgel packings that consist of both soft, loosely crosslinked particles and stiff, densely crosslinked particles, considering packing fractions that cover the range from the onset of particle contact to particles that are strongly packed, deformed, and deswollen. With this strategy, we investigate the transition from a particulate suspension to a macrogel-type system with defined, purposely imparted sub-micrometer scale spatial heterogeneity. We study these inhomogeneous composites from macro- and microscopic perspectives by oscillatory shear rheology and by fluorescence recovery after photobleaching to probe their macroscopic mechanics and the microscopic mobility of flexible linear tracer polymers that diffuse through them.

References: F. Di Lorenzo, S. Seiffert, Macromolecules 2013, 46, 1962. F. Di Lorenzo, S. Seiffert, Colloid Polym. Sci. 2013, 291, 2927.

CPP 52.9 Wed 17:45 C 130

**Dielectric Response of the Water Hydration Layer and its Application on the Solvation Energy** — •Christian Schaaf and Stephan Gekle — University Bayreuth, Bayreuth, Germany

The electric field caused by a charged solute molecule introduced into a dipolar liquid solvent leads to a reorientation of the solvent molecules which is quantified by the solvent's local dielectric constant.

We calculate this dielectric response function using two different methods; linear response for a system with the explicit solute and theoretical calculations using the wave-vector dependent, non-local bulk permittivity. The good agreement leads to our central result: while the water dielectric constant for a radial field in the hydration layer of spherical solutes *is* strongly different from bulk water, this difference is *not* due to significant restructuring of the hydrogen bond network, but can be traced back almost entirely to bulk properties of pure water.

Finally, integrating our dielectric profiles, we calculate the solvation energies for $Na^+$, $Cl^-$, $I^-$, and $Cs^+$ and find quantitative agreement with experimental data.

# CPP 53: Inorganic/organic interfaces: Electronic properties II (joint session O, CPP)

Time: Wednesday 15:00–18:15 Location: HE 101

**Invited Talk** CPP 53.1 Wed 15:00 HE 101
**Electronic structure of Organo-Metal Halide Perovskites Films and Interfaces** — •Antoine Kahn — Princeton University, Princeton, NJ, USA

This talk reviews direct and inverse photoemission data on the electronic structure of organo-metal halide perovskites, i.e., methylammonium lead tri-halides (MAPbX, X=Br3, I3, I3-xClx), and of their interfaces with hole- and electron-transport layers (HTL, ETL). Valence and conduction band edges of the MAPbX films, ionization energy and electron affinity (IE, EA) are determined [1]. Good alignment of the MAPbX conduction band minimum with that of the electron-collecting oxide is found, suggesting minimal energy loss during electron extraction at this interface. The hole-extraction interface is investigated for several HTLs. Results clearly puts into evidence the role of interface energetics in terms of carrier loss-less extraction or confinement in the perovskite layer [2]. The electronic structure of the inverted solar cell, with MAPbI3 on sol-gel processed NiOx, is also investigated [3]. The perovskite takes on a p-type character, indicative of a low density of deep gap states in the material. The NiOx/ MAPbI3 interface energetics provide barrier-free hole extraction (0.2 eV energy loss) and a high electron-blocking barrier. On the other side of the cell, C60 and derivatives form adequate ETLs, with neither a barrier for electron extraction nor a loss in accessible open circuit voltage.

[1] P. Schulz et al., Energ. & Envir. Sci. 7, 1377 (2014) [2] E. Edri et al., J. Phys. Chem. Lett., 5, 429 (2014) [3] P. Schulz et al. (under review)

CPP 53.2 Wed 15:30 HE 101
**Site-specific transport levels in a crystalline organic thin film** — •Tomoki Sueyoshi, Martin Willenbockel, Serguei Soubatch, and Stefan Tautz — Peter Grünberg Institut (PGI-3), JARA, Forschungszentrum Jülich, Germany

Recent studies have revealed that the electronic properties of organic semiconductor thin films are not only determined by the nature of individual constituent molecules, but also correlated with geometric structure in which the molecules arrange. If a crystalline organic thin film consisting of single-component molecules contains several different molecular species in its unit cell, molecular orbital energies of such species could be different from species to species depending on their relative geometry and orientation. Since it is the highest occupied/lowest unoccupied molecular orbitals (HOMO/LUMO) which are involved in charge transport, the energy dispersity of these transport levels may dominate the transport properties of organic semiconductors.

A previous scanning tunneling spectroscopy study revealed that a LUMO energy dispersity up to 0.5 eV originates from the intermolecular polarization/interaction on the LUMO of six different tetracene species in the complex bilayer $\beta$-phase on Ag(111). To access the one on the HOMO, we have performed photoelectron spectroscopy of the tetracene $\beta$-phase and observed a similar energy dispersity of the HOMO. In this talk, we will discuss the assignment of the observed HOMO components and provide a comprehensive picture of the transport levels of the tetracene $\beta$-phase.

CPP 53.3 Wed 15:45 HE 101
**Charge Transport through Molecular Monolayers: Impact of Collective Effects and Docking Groups** — •Veronika Obersteiner$^{1}$, David Egger$^{1,2}$, Georg Heimel$^{3}$, and Egbert Zojer$^{1}$ — $^{1}$Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Graz, Austria. — $^{2}$Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth, Israel. — $^{3}$Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany.

For advancing the exciting field of molecular electronics, a microscopic understanding of charge transport through molecule-based systems is essential. Over the past years, the fundamental physical differences between devices comprising an individual molecule or a homogeneous monolayer have been increasingly acknowledged. Here, we relate those differences to collective electrostatic effects arising from the combined electric fields of all molecules within a monolayer. Employing density functional theory in conjunction with a Green's function approach, we theoretically investigate current-voltage characteristics of metal-molecule-metal systems that comprise either single molecules or an assembly.We show that, depending on the chemical nature of the molecular backbones and the used docking groups, collective effects either significantly increase or decrease the current at a given voltage. As a consequence, the 'ideal' docking group is clearly different for monolayer and single-molecule devices. These insights are also used to design molecules in which collective effects cancel, and thus transport characteristics remain largely unaffected by environmental effects.

CPP 53.4 Wed 16:00 HE 101
**Inverse electron transfer in nitro-substituted monomolecular films** — Prashant Waske$^{1,2}$, •Tobias Wächter$^{1}$, Andreas Terfort$^{2}$, and Michael Zharnikov$^{1}$ — $^{1}$Applied Physical Chemistry, Heidelberg University, 69120 Heidelberg, Germany — $^{2}$Institut für Anorganische und Analytische Chemie, Universität Frankfurt, 60438 Frankfurt, Germany

Self-assembled monolayers of nitro-substituted aromatic thiols were prepared on Au(111) substrates and characterized by several complementary spectroscopic techniques. The introduction of the nitro tail group had a positive effect on the quality of the monolayers, which were either superior or comparable to their non-substituted analogues. All molecules in the films were found to be bound to the substrate via the thiolate anchor and to have an upright orientation. The [N 1s]$\pi^*$ and [O 1s]$\pi^*$ decay spectra of the monolayers did not exhibit any trace of charge (electron) transfer (CT) through the molecular framework to the substrate, following the resonant excitation of the tail group. This was explained by the energy considerations hindering CT to the substrate but enabling a reverse process (ICT), i.e. the neutralization of the core ionized state by electron transfer from the substrate/molecular backbone. Traces of this process could be tentatively identified as an admixture of resonant contributions to the non-resonant decay spectra at the O K-edge. The experimental data suggest that only the ring adjacent to the nitro group was involved in the ICT process.

CPP 53.5 Wed 16:15 HE 101
**Probing single donor-acceptor molecules on thin insulating films** — •Tobias Meier$^{1}$, Rémy Pawlak$^{1}$, Shigeki Kawai$^{1}$, Shi-Xia Liu$^{2}$, Silvio Decurtins$^{2}$, Ernst Meyer$^{1}$, and Thilo Glatzel$^{1}$ — $^{1}$Department of Physics, University of Basel, Switzerland — $^{2}$Department of Chemistry and Biochemistry, University of Bern, Switzerland

Fused Donor-Acceptor molecules have attracted a broad interest due to their potential applications for example in organic solar cells. The intrinsic electronic properties of such organic compounds determine the device performance, notably the intramolecular charge transfers (CT) between the donor and acceptor parts. However, the CT is still poorly understood at the single molecular scale.

In this work we used the TTF-dppz [1], a planar and and pi-conjugated molecule with size of less than 2 nm, adsorbed on thin layers of NaCl on Cu(111). By combining STM and AFM, we spatially characterized the separation of the HOMO and LUMO with respect to the chemical structure of the TTF-dppz molecule observed by AFM. We further investigated with force and current based spectroscopic techniques [2,3] the electronic properties of the molecule and its charge redistribution. To gain more insights into the charge transfer of a single molecule under illumination, we further performed such spectroscopic measurements under illumination.

[1] C. Jia et al., Chemistry 13, 3804 (2007). [2] R. Pawlak et al., Nano Lett. 13, 5803 (2013). [3] S. Kawai et al., ACS Nano 7, 9098 (2013).

CPP 53.6 Wed 16:30 HE 101
**Integer versus fractional charge transfer at metal/organic and metal/insulator/organic interfaces: Cu(/NaCl)/TCNE** — •Oliver T. Hofmann$^{1,2}$, Patrick Rinke$^{1,3}$, Viktor Atalla$^{1}$, Georg Heimel$^{4}$, and Matthias Scheffler$^{1}$ — $^{1}$FHI Berlin, Germany — $^{2}$TU Graz, Austria — $^{3}$Aalto University, Helsinki, Finland — $^{4}$Humboldt University Berlin, Germany

We use semilocal and hybrid density functional theory to study the charge transfer and level alignment at a representative interface between a metal and an organic molecule. To reduce the hybridization strength between the adsorbate and the substrate, we also insert thin insulating NaCl buffer layers. We find that upon direct adsorption on the metal, charge is perfectly delocalized across all molecules, leading to a laterally homogenous layer. However, when the hybridization between metal and organic is prevented by an insulating interlayer, charge localizes on individual moieties, creating laterally inhomogenous charge distributions. This spontaneous breaking of the translation symmetry is reflected in several observables, such as the molecular geometry or the valence and core densities of states. We find that the amount of charge transfer is determined, to a significant extend, by the ratio of the lateral spacing of the molecules and their energetic distance to the electron reservoir, i.e., the metal. Therefore, the amount of charge transfer does not only depend on the electronic structure of the individual components, but also on the interface geometry. Furthermore, we discuss the impact of the lateral charge distribution on the coverage dependence of the work function for different growth models.

CPP 53.7 Wed 16:45 HE 101

**Controlled photo-induced work function manipulation of the TCNQ/Au(111) interface** — •David Gerbert and Petra Tegeder — Physikalisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg, Germany

One of the most important tasks to improve the performance of organic electronic devices is the development of deeper understanding and purposeful employment of metal electrode*s work function manipulation [1]. In the first layer TCNQ is known to be negatively charged on various metal surfaces [2,3], however only on Au(111) it is neutral [4]. We investigated the electronic structure of the TCNQ/Au(111) interface by means of two-photon-photoemission (2PPE) and observed a photo-induced work function shift of several hundred meV, which points towards photo-induced electron transfer from the gold substrate to the molecule. Interestingly the work function can be continuously tuned across the clean surface value which establishes new application possibilities of TCNQ as device-adapted hole-injection layer.

[1] N. Koch, ChemPhysChem. 8, 1438-1455 (2007).

[2] C. Park et al., Phys. Rev. B 90, 125432 (2014).

[3] T.-C. Tseng et al., Nat. Chem. 2, 374 (2010).

[4] I. Fernandez-Torrente et al., Int. J. Mass Spectrom. 277, 269-273 (2008).

CPP 53.8 Wed 17:00 HE 101

**The geometric and electronic structure of TCNQ and TCNQ+Mn on Ag(001) surface** — Vitaliy Feyer[1], Martin Graus[2,3], •Giovanni Zamborlini[1], Robert G. Acres[4], Achim Schöll[2,3], Friedrich Reinert[2,3], and Claus M. Schneider[1,5] — [1]Research Center Jülich, 52425 Jülich, Germany — [2]Universität Würzburg, Experimentelle Physik VII & Röntgen Research
Center for Complex Material Systems RCCM, 97074 Würzburg, Germany — [3]Karlsruher Institut für Technologie KIT, Gemeinschaftslabor für Nanoanalytik, 76021 Karlsruhe, Germany — [4]Sincrotrone Trieste, 34012 Basovizza, Trieste, Italy — [5]Universität Duisburg-Essen, D-47048 Duisburg, Germany

We have investigated the geometric and electronic structure of ordered monolayers of TCNQ and of TCNQ+Mn on Ag(001) surface by LEED and photoelectron momentum microscopy (at the NanoESCA beamline of the Elettra synchrotron). Two coverage dependent, commensurable superstructures are established on Ag(001) while the coadsorption of Mn results in the formation of a long-range ordered mixed metal-organic superstructure, which is also commensurate. From ARPES pattern of the TCNQ LUMO the azimuthal orientation of the molecules in the respective unit cell can be determinate. The PES data shows, in the case of TCNQ/Ag(100) a filling of the TCNQ LUMO by charge transfer from the substrate while the coadsorption of Mn leads to an energy shift of the TCNQ HOMO and LUMO of 230 meV with respect to TCNQ/Ag(001). No significant lateral band dispersion in the adsorbate layers was observed in ARPES data.

CPP 53.9 Wed 17:15 HE 101

**Adsorption and electronic properties of tetraazaperopyrene derivatives on Au(111)** — •Friedrich Maass[1], Stephan Stremlau[1], Lena Hahn[2], Lutz H. Gade[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg, 69120 Heidelberg, Germany — [2]Anorganisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg, 69120 Heidelberg, Germany

The adsorption behavior of large N-heterocyclic pi-conjugated molecules is of immense interest for understanding the structural and electronic properties of this new class of organic n-channel semiconductors.

We investigated the adsorption geometry and the electronic properties of 1,3,8,10-tetraazaperopyrene (TAPP) and its 2,9-bisperfluoroalkyl-4,7,11,14-tetra-X derivatives (X is H, Cl, Br or I) on the Au(111) surface with vibrational and electronic high resolution electron energy loss spectroscopy (HREELS) and thermal desorption spectroscopy (TDS). We found a different adsorption behavior between substituted and unsubstituted TAPP and also between monolayer and corresponding multilayers. HOMO-LUMO gaps have been investigated by electronic HREEL spectroscopy and are in good agreement with previously made UV/VIS and calculated data.

CPP 53.10 Wed 17:30 HE 101

**Effects of embedded dipole in alkanethiolate self-assembled monolayers** — Swen Schuster[1], Nichole Sullivan[2], Orlando Cabarcos[2], Iris Hehn[3], Jean-François Morin[4], Egbert Zojer[3], David L. Allara[2], and •Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany — [2]Department of Chemistry, Pennsylvania State University, University Park, PA 16802, USA — [3]Institute of Solid State Physics, Graz University of Technology, 8010 Graz, Austria — [4]Département de chimie, Faculté des sciences et de genie, Université Laval, Québec QC G1V 0A6, Canada

Self-assembled monolayers (SAMs) bonded to metal electrodes are capable to improve charge-carrier injection across the metal-organic interface. This is usually achieved by use of the terminal dipolar groups (terminal dipole) comprising the outer interface of SAMs. But such an architecture affects the growth mode of an organic semiconductor (in the standard device configuration) entangling it with the dipole control. In contrast, for the molecules with an embedded dipolar element, the dipole control and the chemistry at the SAM-ambience interface are decoupled. In this context, we studied a series of SAMs prepared on Au{111} from the mid-chain ester functionalized alkanethiols. The presence of the ester moiety leads to interesting electrostatic effects in photoemission and allows to modify the work function of the substrate in a certain range. The results are rationalized with a help of theoretical simulations, involving a combination of DFT and molecular dynamics methods.

CPP 53.11 Wed 17:45 HE 101

**The Role of Pauli-Pushback fort he Electronic Properties of Self-Assembled Monolayers at Reduced Coverage** — •Elisabeth Verwüster[1], David A. Egger[1,2], Oliver T. Hofmann[1], and Egbert Zojer[1] — [1]Institute of Solid State Physics, Graz University of Technology, NAWI Graz, Petersgasse 16, 8010 Graz, Austria — [2]Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel

Using density-functional theory, advanced geometry optimization tools and accounting for van der Waals interactions we explain the coverage-dependent electronic structure of self-assembled monolayers (SAMs). As model systems for our calculations we choose acceptor- (-CN, -CF3) and donor- (-CH3, -NH2) substituted biphenylthiols on a Au(111) surface. Our focus lies on changes in the SAM-induced work-function modification, $\Delta\Phi$. Upon reducing the coverage the tilt angle of the molecules strongly increases. The latter significantly affects the molecular dipole perpendicular to the surface. The resulting changes in $\Delta\Phi$ are, however, much more pronounced than one could expect on purely geometric grounds. For example, $\Delta\Phi$ vanishes already at a coverage of 50% for the acceptor-substituted SAMs. This can only partly be explained by the tilt-angle dependence of the charge-rearrangements arising from the S-Au bond formation. Instead, we show that especially at low coverage the interaction-induced charge-rearrangements at the interface are dominated by Pauli-pushback, an effect well known for flat-lying adsorbates.

CPP 53.12 Wed 18:00 HE 101

**Electrostatic design of monolayer properties** — Bernhard Kretz[1], David A. Egger[1,2], and •Egbert Zojer[1] — [1]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria — [2]Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel

For raising the full potential of molecular electronics, it is necessary to control the nature of the electronic states within organic layers. In this contribution we present the concept of a modular toolbox that allows realizing a high level of control as far as the energetics and spatial localization of the states is concerned. By quantum-mechanical modelling we show that - based on this toolbox - it is, for example, possible to realize monolayer-based quantum-cascades and electron or hole quantum-well structures. This becomes possible by exploiting collective electrostatic effects naturally emerging in ensembles of polar molecules. As another element of the toolbox we discuss neutral radicals that can be applied for generating locally spin-polarized layers.

# CPP 54: Wetting, Micro and Nanofluidics (joint session CPP, DY)

Time: Wednesday 15:00–18:15 Location: C 243

CPP 54.1 Wed 15:00 C 243

**Lateral adhesion force of superhydrophobic surfaces** — •Doris Vollmer, Dominik Pilat, Nan Gao, Periklis Papadopoulos, Frank Schellenberger, Rüdiger Berger, and Hans-Jürgen Butt — MPI for Polymer Research, Mainz, Germany

We designed an instrument to measure the lateral adhesion force of drops on surfaces (1). The forces required to slide a sessile drop over a surface was measured by means of the deflection of a capillary that stuck in the drop. This allows the investigation of the dynamic lateral adhesion force of water drops on superhydrophobic surfaces. The movement of the drop relative to the surfaces enabled us to resolve the pinning of the three-phase contact line. This was related to the shape of the drop profile, which was recorded by video microscopy. The lateral adhesion of a drop on a superhydrophobic pillar array was quantified in dependence of pillar spacing and drop velocity.

(1) D.W. Pilat, P. Papadopoulos, D. Schaeffel, D. Vollmer, R. Berger, and H.-J. Butt, Langmuir 2012, 28, 16812.

CPP 54.2 Wed 15:15 C 243

**Drying and Wetting transitions on irregular rough substrates.** — •Segun Gideon Ayodele, Ciro Semprebon, Renaud Dufour, Stephan Herminghaus, and Martin Brinkmann — Max-Planck Institut für Dynamik und selbstorganisation, 37077 Göttingen.

Drying and wetting transitions on non-flat solids of homogeneous wettability are studied employing a sharp interface model. Interfacial configurations in the Grand canonical ensemble and corresponding numerical energy minimizations for a non-zero microscopic contact angle are compared to predictions based on the statistical model proposed in Refs. [1,2]. This mean field model considers exclusively local descriptors of the substrate topography such as the distribution of heights, as well as averages of the slope and its square at a given height. In contrast to the continuous desorption isotherm of a zero microscopic contact angle, we observe an increasingly discontinuous decay of the average film thickness in our numerical simulations during a desorption as the microscopic contact angle is increased. The pressure of the final drying transition as observed in the simulated annealing and numerical energy minimization is in agreement with predictions of the 'Wenzel prewetting' transition in the mean field model [1,2].

1. S. Herminghaus, Eur. Phys. J. E 35, 43 (2012).
2. S. Herminghaus, Phys. Rev. Lett., 109,236102 (2012).

CPP 54.3 Wed 15:30 C 243

**Dynamic Trapping of Sliding Drops on Wetting Defects** — •Andrea Cavalli[1], Michiel Musterd[2], Rudy Lagraauw[1], Dieter 't Mannetje[1], Dirk van den Ende[1], and Frieder Mugele[1] — [1]University of Twente, MESA+ Institute for Nanotechnology; Physics of Complex Fluids, Enschede, The Netherlands — [2]Delft University of Technology, Delft, The Netherlands

We present a numerical analysis of the dynamic interaction of sliding drops on an inclined plate with wetting defects. Our three-dimensional model, developed with OpenFOAM allows us to describe intertial and viscous effects, as well as the internal degrees of freedom of the droplet. We observe that the ability of a drop to deform and stretch enhances the strenght and range fo the wetting defect, as compared to a simplified analytic description of a non-deformable drop. Yet, the key physical parameters, namely the ration between trapping strength and driving force as well as the ratio between interial and viscous time scale prevail as governing control parameters. We further investigate the role of the strength, size and steepness of the wetting defect in retaining the drop. Finally, we compare our simulations with trapping experiments on electrowetting obstactles. The quantitative agreement shows that the trapping of sliding drops follows a universal behavior, which is largely independent of the specific nature of the defect.

CPP 54.4 Wed 15:45 C 243

**Sub-nanometric substrate structural changes enhance the solid/liquid slip boundary condition** — •Joshua McGraw, Antoine Bridet, Samuel Grandthyll, Hendrik Hähl, Frank Müller, and Karin Jacobs — Experimental Physics, Saarland University, 66041 Saarbrücken, Germany

Alkylsilane self-assembled monolayers (SAMs) have long been used as model substrates for their ease of preparation and hydrophobic properties. We have long observed that these monolayers also provide a slip boundary condition for dewetting polymer films, and that the slip condition is switchable if the alkyl chain length is changed (from 12 to 18 backbone carbons, for example). Typically, this change is affected in a quantized way, using one or the other chain length, thus obtaining one or the other slip condition. It has been suggested that the specific structure of the resulting SAM controls the slip condition. Here, we present results in which this structure is changed in two continuous ways. First, we prepare SAMs containing bidisperse mixtures of alkyl silanes, with the composition as a control parameter. Second, we thermally anneal the SAMs, resulting in an irreversible loss of carbon from the monolayer. In both cases, we find an enhanced slip condition which is tuneable over a certain range.

CPP 54.5 Wed 16:00 C 243

**Universal Regimes in the Relaxation of Stepped Liquid Interfaces near Contact Lines** — •Marco Rivetti[1], Thomas Salez[2], Michael Benzaquen[2], Elie Raphael[2], and Oliver Baeumchen[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Goettingen, Germany — [2]Laboratoire de Physico-Chimie Theorique, UMR 7083 CNRS & ESPCI ParisTech, Paris, France

A liquid droplet on a perfectly smooth surface wets or dewets the substrate according to the difference between initial and equilibrium contact angles [1]. Such a scenario, however, becomes less intuitive whenever the initial shape of the interface is non-spherical. Indeed, the capillary-driven relaxation of the liquid surface may be in competition with the relaxation of the contact angle at the three-phase contact line. Here, we study the dynamics of stepped interfaces of thin polystyrene films on hydrophilic substrates. Annealing the polymeric film above its glass transition temperature induces flow which is precisely monitored using ex- and in-situ atomic force microscopy. Both pinned and receding contact line regimes are observed. Rescaling with regard to the viscosity, surface tension and film thickness collapses the data on a master curve, providing a universal time for the transition between both regimes. In addition, we prove that the pinned interface exhibits self-similar height profiles which are captured by a thin film model in lubrication approximation [2].

[1] S.L.Cormier et al, PRL 109, 154501 (2012); [2] J.D.McGraw et al, PRL 109, 128303 (2012)

CPP 54.6 Wed 16:15 C 243

**Dynamic Contact Angle of a Soft Linear Viscoelastic Solid** — •Stefan Karpitschka[1], Siddhartha Das[2], Mathijs van Gorcum[1], Hugo Perrin[3], Bruno Andreotti[3], and Jacco H. Snoeijer[1,4] — [1]Physics of Fluids Group, Faculty of Science and Technology, Mesa+ Institute, University of Twente, 7500 AE Enschede, The Netherlands — [2]Department of Mechanical Engineering, University of Maryland, College Park, MD 20742, USA — [3]Physique et Mécanique des Milieux Hétérogènes, UMR 7636 ESPCI -CNRS, Univ. Paris-Diderot, 10 rue Vauquelin, 75005, Paris, France — [4]Department of Applied Physics, Eindhoven University of Technology, P.O. Box 513, 5600MB Eindhoven, The Netherlands

The wetting motion of a liquid over a rigid solid gives rise to a dynamic liquid contact angle. Here we show that on a soft, viscoelastic substrate, a moving contact line leads to a dynamic contact angle of the solid. The initially flat solid surface is deformed elastically into a sharp ridge. The ridge shape and the orientational angle of its tip depend on the contact line velocity. We present a theory based on linear response that reveals how the dynamics of the wetting ridge emerges from the substrate rheology. The theory is validated experimentally with measurements of the dynamic contact angle on a silicone gel.

**15 min. break**

CPP 54.7 Wed 16:45 C 243

**Capillary force acting on a particle correlated with the shape of the meniscus** — •Frank Schellenberger, Periklis Papadopoulos, Stefan Weber, Michael Kappl, Doris Vollmer, and Hans-Jürgen Butt — Max Planck Institute for Polymer Research, Mainz, Germany

Capillary bridges play a important role for the stability of colloidal systems. The forces of these bridges strongly correlates with their shape. It is possible to measure capillary forces with an Atomic Force Microscope (AFM), but it is impossible with such a device to image the shape of the capillary bridge at the same time.

Analytical and numerical calculations exist that correlates the force of the capillary bridges with the shape of the liquid . However experimentally capillary bridges could not directly be imaged with the corresponding force in the micrometer range so far. A Laser Scanning Confocal Microscope (LSCM) can visualize the shape of a liquid bridge on solid surface in a three-dimensional form. We built a combined LSCM and AFM device and measured the forces with colloidal probes on liquid surfaces. The combination of force spectroscopy and confocal microscopy allows us to image capillary bridges and simultaneously measure the corresponding force.

With our setup we can now verify the theoretical forces, calculated from the shape of the meniscus, and the corresponding force curves. We present our results of the simultaneous AFM and LSCM measurements of capillary bridges.

CPP 54.8 Wed 17:00 C 243

**Wettability-independent bouncing on flat surfaces** — Jolet de Ruiter, Rudy Lagraauw, Dirk van den Ende, and •Frieder Mugele — University of Twente; MESA+ Institute for Nanotechnology, Physics of Complex Fluids, Enschede, The Netherlands

The impingement of drops onto solid surfaces plays a crucial role in a variety of processes, including inkjet printing, fog harvesting, anti-icing, dropwise condensation and spray coating. Recent efforts in understanding and controlling drop impact behaviour focused on superhydrophobic surfaces with specific surface structures enabling drop bouncing with reduced contact time. Here, we report a different universal bouncing mechanism that occurs on both wetting and non-wetting flat surfaces for both high and low surface tension liquids. Using high-speed multiple-wavelength interferometry, we show that this bouncing mechanism is based on the continuous presence of an air film for moderate drop impact velocities. This submicrometre air cushion slows down the incoming drop and reverses its momentum. Viscous forces in the air film play a key role in this process: they provide transient stability of the air cushion against squeeze-out, mediate momentum transfer, and contribute a substantial part of the energy dissipation during bouncing.

CPP 54.9 Wed 17:15 C 243

**Surfactants in droplet-based microfluidics – Adsorption, Exchange and Biocompatibility** — •Birte Riechers[1,2], Philipp Gruner[2], Florine Maes[1,2], and Jean-Christophe Baret[1,2] — [1]Center de Recherche Paul Pascal, Bordeaux, France — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Emulsions are omnipresent in industry, research and daily life. They are widely used in painting materials, cosmetics as well as for medical and biotechnology applications [Bremond et al. Soft Matter 2012]. Emulsions are multiphase liquids stabilised using surfactants. These amphiphilic molecules adsorb to interfaces changing their properties (e. g. surface tension, interfacial rheology) [Baret Lab Chip 2012]. They also chemically or physically interact with the dispersed aqueous phase effecting solubility of solutes in all phases [Skhiri et al. Soft Matter2012].

Here, we analyse the properties of surfactants which result in undesirable reactions and interactions with the interior of the droplets. We present a microfluidic method to determine the adsorption kinetics of surfactants. The principle is based on miniaturised pH measurements at the micron-scale. We show that the surfactant exchange between the droplet interface and the continuous phase occurs within seconds and significantly effects the loss of chemicals from droplets. Our method provides new means to analyse surfactant interfaces and their interactions with the aqueous phase of emulsion droplets. We anticipate that our approach can be used to optimise surfactants and formulations for applications in emulsion-based biochemical analysis.

CPP 54.10 Wed 17:30 C 243

**Coexistence of Various Instabilities on a Single Liquid Filament** — Michael Hein[1], •Jean-Baptiste Fleury[1], and Ralf Seemann[1,2] — [1]Saarland University, Experimental Physics, Saarbruecken, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany

Droplet based microfluidics exploits the decay of a liquid filament or cylinder into droplets of micrometric size. While the physics of droplet breakup on small scales remains a field of vivid interest, droplet based microfluidic systems have become widely used both in fundamental science and application such as (bio-)analytics or micro-chemistry. We present experimental research on the formation of droplets by breakup of a squeezed liquid filament surrounded by an immiscible phase that flows over a topographic step. This non-equilibrium process arises from the interplay between flow properties and interfacial instabilities when the filament is suddenly released from confinement at the step. In contrast to previous studies, a rich variety of different droplet breakup regimes was observed for the used geometry which are characterized by the coexistence of multiple liquid instabilities on a single filament. Surprisingly, these instabilities can be of different type while the filament is exposed to a symmetric flow-field. This spontaneous symmetry breaking is a nontrivial consequence of volume throughput constraints of each individual instability and allows for the specific production of heterogeneous droplet families from one single filament under constant flow rates.

(Michael Hein, Jean-Baptiste Fleury and Ralf Seemann, Submitted)

CPP 54.11 Wed 17:45 C 243

**Inertial microfluidics: control of lift forces and dynamics of microfluidic crystals** — •Christopher Prohm and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin

At intermediate Reynolds numbers, particles in microfluidic channels assemble at fixed distances from the channel axis and bounding walls [1]. This Segré-Silberberg effect can be described in terms of an inertial lift force acting on the particles. At increasing densities the particles form microfluidic crystals due to an interplay of hydrodynamic interactions and inertial lift forces [2]. Microfluidic devices utilizing inertial migration have recently been demonstrated for biomedical tasks such as particle sorting or separation [1].

Here, we investigate the motion of colloidal particles in microfluidic channels using the lattice Boltzmann method [3]. First, we show how the geometry of the channel influences inertial focusing of a single particle. We also demonstrate that manipulating the axial or angular velocity of the particle modifies its lift-force profile, which permits control of the lateral particle position. Second, we investigate suspensions of particles. We describe how they self-assemble into microfluidic particle crystals and discuss the dynamic properties of these crystals.

[1] H. Amini, W. Lee, and D. Di Carlo, *Lab Chip* **14**, 2739 (2014).

[2] W. Lee, H. Amini, H. A. Stone, and D. Di Carlo, *Proc. Natl. Acad. Sci. U.S.A.* **107**, 22413 (2010).

[3] C. Prohm and H. Stark, *Lab Chip* **14**, 2115 (2014).

CPP 54.12 Wed 18:00 C 243

**High-throughput and passive trapping of nano-objects using electrostatic forces** — •Michael Adrian Gerspach[1,2,3], Nassir Mojarad[2], Yasin Ekinci[2], and Thomas Pfohl[1,3] — [1]Swiss Nanoscience Institute, Basel, 4056, Switzerland — [2]Paul Scherrer Institute, Villigen, 5323, Switzerland — [3]Department of Chemistry, University of Basel, Basel, 4056, Switzerland

Contact free trapping of nano-objects in solution is of broad interest. Although several methods have been developed, like optical tweezers, stable and high throughput trapping of nanometer-sized particles remains challenging. Our approach of trapping charged nano-objects is geometry induced electrostatic trapping [1], a method based on altering the surface topology of nano-channels that are negatively charged when exposed to water. Here we present the on chip contact free trapping of single 40 to 80 nm gold particles in nanometer-sized pockets without the use of any externally applied forces. The particles in the solution are pushed into the pockets and trapped only because of the difference in electrostatic potential between the nanofluidic channel walls and the finer pocket structures. Increasing the salt concentration of the solution leads to screening of the surface charges by free counter ions and therefore, weakens the trap strength and shortens the average time a particle dwell in a trap. Thus by chancing the concentration of the solution or the height of the nanofluidic channels, the particles can be trapped from microseconds to several minutes. In future we plan to extend this method to trap and investigate the dynamics of biological entities such as DNA or large proteins. [1] Nature 457 (2010), 692-695

## CPP 55: Flow-Induced Structures in Complex Fluids (with DRG, Deutsche Rheologische Gesellschaft, and DY)

Annual Meeting of the German Rheological Society together with the Spring Meeting of the Condensed Matter section of German Physical Society

Time: Wednesday 15:00–18:30 Location: C 264

**Invited Talk** CPP 55.1 Wed 15:00 C 264

**A new perspective of materials processing** — •Kyung Hyun Ahn — Seoul National University, Seoul, Korea

With recent advances in emerging technologies, materials design encounters new challenges. With more nano particles inside, processing experiences thinner and faster deformations than ever, which should be reflected in materials design. However, little is known about the flow characteristics of such complex fluids and less is known about how to design and control the process. Industrial coating materials such as ink, slurry and paste form heterogeneous microstructure as they contain various components. Therefore, it is necessary to incorporate the concept of heterogeneity into materials processing and to develop the methodology to quantitatively analyze the heterogeneous nature observed in both materials and processing. It will be a big challenge to establish a systematic protocol to characterize the materials and maintain uniform quality during manufacturing. In this talk, I will show illustrative examples that prove the heterogeneous nature in different length scales, covering the length scale from nano, micro to macro. With many illustrative examples of both system and methodology, I will deliver my idea on the perspective and strategy of the researches, which will be a new paradigm of materials processing as well as of materials design.

CPP 55.2 Wed 15:30 C 264

**Slow dynamics in sheared DGEBA/$SiO_2$ suspensions** — •Rick Dannert, Roland Sanctuary, and Jörg Baller — University of Luxembourg, Laboratory for the Physics of Advanced Materials, Grand-Duchy of Luxembourg

Investigations of concentrated and semi-diluted colloidal suspensions of spherical silica nanoparticles in Diglycidyl Ether of Bisphenol A (DGEBA) with oscillatory shear rheology have recently shown an anomaly at low frequencies, which was interpreted as Brownian stress relaxation resulting from strain-induced perturbations of the isotropic filler distribution [1]. To complete the study of the concentration dependency we extend the rheological investigation of the low-frequency anomaly to ultra-diluted DGEBA/silica suspensions. We illustrate that the Brownian relaxation process depends in a complex manner on the volume concentration: the relaxation frequency exhibits a maximum at low filler contents. This non-monotonic dependency of the relaxation frequency can no longer be modelled by classical Peclet frequencies. Including a structural, concentration dependent parameter allows for an accurate description of the Brownian relaxation process for all concentrations.

[1] R. Dannert, R. Sanctuary, M. Thomassey, P. Elens, J.K. Krüger, J. Baller, Rheologica Acta, 53 (2014) 715-723.

CPP 55.3 Wed 15:45 C 264

**Microstructure and nonlinear signatures of yielding in a heterogeneous colloidal gel under large amplitude oscillatory shear** — Juntae Kim[1], •Dimitri Merger[2], Manfred Wilhelm[2], and Matthew E. Helgeson[1] — [1]Department of Chemical Engineering, University of California Santa Barbara, Santa Barbara, California 93106 — [2]Institute for Chemical Technology and Polymer Chemistry, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

We investigate yielding in a colloidal gel that forms from a nanoemulsion by polymer mediated aggregation. Combining large amplitude oscillatory shear measurements with simultaneous small and ultra-small angle neutron scattering (rheo-SANS/USANS), we characterize both the nonlinear mechanical processes and strain amplitude-dependent microstructure underlying yielding. We observe a broad, three-stage yielding process that evolves over an order of magnitude in strain amplitude between the onset of nonlinearity and flow. Analyzing the intracycle response stress reveals a transition from elastic straining to elastoplastic thinning which eventually leads to yielding and flow. The instantaneous nonlinear parameters associated with yielding are correlated with time-averaged rheo-USANS measurements. This shows how the material passes through a cascade of structural breakdown from large to progressively smaller length scales. All significant structural changes occur on the micron-scale, suggesting that large-scale rearrangements of hundreds or thousands of particles, rather than the homogeneous rearrangement of particle-particle bonds, dominate the initial yielding of heterogeneous colloidal gels.

CPP 55.4 Wed 16:00 C 264

**Rheological behavior of a highly concentrated colloidal dispersion on different length scales** — •Clara Weis and Norbert Willenbacher — Karlsruhe Institute for Technology (KIT), Karlsruhe, Germany

Multi particle tracking and bulk mechanical rheometry have been used to study rheological properties of concentrated, colloidal suspensions. Using fluorescent tracer particles with particle sizes between 100nm and 1000nm enables MPT even in turbid systems and provides rheological information on the microscale. Following systems have been investigated: 1. Fluid suspensions with short range repulsive interactions at $\Phi$eff<0.5, in this case perfect agreement between bulk and microrheology is found. 2. Hard sphere type crystallizing dispersions in the liquid/crystalline coexistence regime with and without added non-adsorbing polymer. A large variation in mean square displacement (MSD) of different tracer particles with slopes $\delta$MSD/$\delta\tau$ between 0 and 1 is found. The heterogeneity of the samples can be directly imaged based on this rheological contrast. The broadening of the coexistence region due to weak attractive depletion forces induced by added polymer is directly proven by MPT. 3. Variation of tracer particle mobility is investigated for systems approaching the colloidal glass transition. 4. The change of particle mobility and the variation of sample heterogeneity is analyzed in the so-called re-entry regime at $\Phi$>$\Phi$g = 0.58 where the system transitions from glassy to fluid and from fluid to gel-like when attractive interaction controlled by non-adsorbing polymer increases from 0 to about 10 kT.

CPP 55.5 Wed 16:15 C 264

**Microstructural studies of colloidal glasses using forced probe particles** — •Markus Gruber[1], Gustavo Abade[1], Antonio Puertas[2], and Matthias Fuchs[1] — [1]Universität Konstanz, Germany — [2]Universidad de Almería, Spain

Driving a colloidal probe particle through a complex fluid provides unique insights into local viscoelastic properties. For soft solids there is a delocalization transition when the force on the probe particle is large enough to pull it free [1]. We study the spatial probability distribution of a tracer particle as seen by active microrheology in constant force mode. As model system, we consider a bath of hard spheres performing Brownian motion in the glassy state and an actively pulled hard sphere tracer particle. The spatial probability distribution is accessed within mode-coupling theory (MCT) refining the previous model [2] by decomposing the mobility-tensor kernel as suggested by [3] to obtain physical results for even larger forces.

Highly nonlinear effects for example in mean and mean square displacements are seen already below the critical force. One reason is the emergence of an exponential tail of the probability distribution in the direction of the applied force, which can also be found in molecular dynamic computer simulations (MDS). In addition we compare other MCT predictions with results from MDS.

[1] I. Gazuz, et al. Phys. Rev. Lett. 102 (2009) 248302.
[2] Ch. J. Harrer, et al. Z. Phys. Chem. 226 (2012) 779.
[3] S. Lang et al. J. Stat. Mech. P12007 (2013).

CPP 55.6 Wed 16:30 C 264

**Rheological properties of temporarily cross-linked microcapsules** — •Sarah Demand and Heinz Rehage — Chair of Physical Chemistry II, TU Dortmund, 44227 Dortmund, Germany

Microcapsules have a broad spectrum of different applications and can be used as simple model systems for understanding the mechanical properties and controlled release processes of biological cells, e. g. erythrocytes. Capsules consist of a tiny fluid droplet which is surrounded by an ultra-thin, flexible membrane. Temporary networks, which simply emerge from self-organization processes of surfactants, are of special interest. These coherent films exhibit striking viscoelastic properties which are influenced by dynamic fluctuations and the average life-time of cross-linking points. A typical emulsifying compound, showing this special ambivalent behavior, is the polysaccharide surfactant Span 65. In order to measure the kinetics of crosslinking and the stability of Span 65-films, we performed different types of rheological investigations. The shear and dilatational behavior of microcapsules was obtained from deformation studies in external fields. Capsule deformations in centrifugal fields were studied in a spinning-drop tensiometer. The deformation and orientation behavior in simple shear flow was investigated by means of an optical rheoscope. The results of all the studies showed a high ability of temporarily cross-linked surfactant films to stabilize emulsion droplets. Due to their processes of self-organization, this provides new and interesting perspectives for simple and effective micro- and nano-capsule technologies.

CPP 55.7 Wed 16:45 C 264

**Clusters formation in microcirculation** — Othmane Aouane[1,2,3], Marine Thiebaud[2], Chaouqi Misbah[2], and •Christian Wagner[1] — [1]Department of Experimental Physics, Saarland University, 66123 Saarbrücken, Germany — [2]Université Grenoble Alpes, LIPHY, F-38000 Grenoble, France — [3]LMPHE, URAC 12, Faculte des Sciences, Rabat, Morocco

We investigate numerically the flow of deformable objects such as vesicles and red blood cells (rbcs) in micro-channels. We focus on understanding the phenomena behind the formation of small train of cells (called clusters) that occurs in the microcirculation. We consider the rbc in 2D as a closed deformable and non-permeable membrane encapsulating an inner fluid and suspended in an outer fluid. The membrane total force is composed from a bending force, a tension force to fulfill the area conservation constraint, and a cell-cell interaction force to reproduce the depletion forces due to the effect of the plasma macromolecules such as fibrinogen. The cells are placed in a confined geometry (two parallel walls) and subjected to a Poiseuille flow. The inner and outer fluids obey to Stokes equations. This equations are solved using the boundary integral formulation. We observe that two kind of clusters exist namely: i) hydrodynamical clusters, and ii) polymer induced clusters. We notice that there is an interplay between the confinement and the formation/destruction of hydrodynamical clusters. The polymer induced clusters are more robust and remain stable independently from the confinement.

**15 min. break.**

CPP 55.8 Wed 17:15 C 264

**Red blood cells in intimate contact** — •Achim Guckenberger and Stephan Gekle — Biofluid Simulation and Modeling, University of Bayreuth, Germany

Red blood cells in confined flow exhibit an effective hydrodynamic attraction: At low volume fractions, they tend to form pairs of cells (clusters). Understanding this effect is important for designing microfluidic devices. Furthermore, agglomeration of erythrocytes plays a major role in biological processes ranging from clotting to cardiovascular diseases. We study this phenomenon with the help of a three-dimensional periodic boundary integral method for various parameter sets. Amongst other things, the cell to cell distance is found to depend on the channel geometry and the flow rate. However, it is independent of the initial configuration of the cells.

CPP 55.9 Wed 17:30 C 264

**Flow of complex fluids into porous media** — •Viviane Lutz Bueno[1], Marianne Liebi[2], and Peter Fischer[1] — [1]ETH, Zürich, Switzerland — [2]Paul Scherrer Institute, Villigen, Switzerland

The dynamic behavior of complex fluids is studied by controlling flow-geometry-fluid interactions. Quantitative information on flow-induced structures (FIS) and in-situ rheological response are reported. Wormlike micelles (WLMs) flowing through porous media lead to a highly transient and localized rheological signature, composed by shear-banding and FIS due to micellar alignment, stretching, and breaking down. The porous media is simplified by a single contraction for initial studies on shear/extensional rates, microstructure organization, and velocity fields. Flow confinement provokes shear banding and viscoelastic instabilities, which dependent on channel's geometry. Micro-designed channels provide extreme fluid confinement and tailored flow-geometry, which are investigate by flow-induced birefringence, micro-particle image velocimetry, and scanning small-angle x-ray/neutron scattering. High shear/extensional rates in the flow through an array of cylinders cause permanent fluid gelation. By decoupling extensional and shear contributions, some of the critical factors, which influence this FIS formation, are reported.

CPP 55.10 Wed 17:45 C 264

**A thermodynamic study of shear banding in polymeric solutions** — •Natalie Germann — Technische Universität München, Freising, Deutschland

Shear banding is an ubiquitous phenomenon occurring in soft matter. The mechanisms behind this type of flow instability is not fully understood. It has been hypothesized (1) that the formation of localized shear bands in polymeric solutions is caused by the diffusion of the polymers. In the first part of this talk, we will introduce a new model for polymeric solutions. A new thermodynamically consistent two-fluid approach (2-3) was employed to account for Fiction diffusion and shear-induced migration effects. In this two-fluid approach, the differential velocity resulting from local variations in concentration and conformation is treated as a state variable. The additional boundary conditions arising from the spatial derivatives of the diffusion terms in the time evolution equations are now directly imposed with respect to that state variable. Hence, it is not anymore necessary to make assumptions about the polymeric microstructure on the boundaries. In the second part of this talk, we will discuss the transient behaviour of the model. The influence of the viscoelasticity of the polymers and the flow geometry on the shear band formation will be examined. The uniqueness of the numerical results and the conditions under which multiple banded states develop will also be elaborated. (1) M. Cromer, G.H. Fredrickson, and L.G. Leal, Phys. Fluids, 26, 063101, 2014. (2) N. Germann, L.P. Cook, and A.N. Beris. JNNFM, (207):21-31, 2014. (3) N. Germann, L.P. Cook, and A.N. Beris, in preparation.

CPP 55.11 Wed 18:00 C 264

**Evidence for simultaneous appearance of gradient and vorticity shear bands using time-resolved Rheo-SANS and laser light transmittance measurements** — •Annekathrin Mütze[1], Peggy Heunemann[1], Lionel Porcar[2], and Peter Fischer[1] — [1]ETH Zürich, Schmelzbergstr. 9, 8092 Zürich, Switzerland — [2]Institute Laue-Langevin, 6 rue Jules Horowitz, B.P.156, F-38042 Grenoble Cedex 9, France

The flow properties of wormlike micellar surfactant solutions play an important role in applications like drag reduction in turbulent flows, fracturing fluids, and encapsulation agents. Such systems are studied with respect to the applied shear stress, concentration, temperature and composition of the salt counter ions. A combination of rheological measurements, laser-light transmittance, video analysis, and rheo-small angle neutron scattering allow a detailed exploration of number and types of shear bands. Typical flow curves of the solutions show Newtonian, shear-thinning, and shear-thickening flow behavior. In the latter regime, the solutions show vorticity and gradient shear bands simultaneously, in which vorticity shear bands dominate the visual effect, while gradient shear bands always coexist and predominate the rheological response. We show that gradient shear bands change their phases (turbid, clear) with the same frequency as the shear rate oscillates, whereas in-time vorticity shear bands change their phases with half the frequency of the shear rate [1].

[1] A. Mütze, P. Heunemann, P. Fischer. Journal of Rheology 58(6): 1647

CPP 55.12 Wed 18:15 C 264

**Soft Solid Rheology Near the Gel Point** — •Horst Henning Winter — University of Massachusetts Amherst

For most amorphous materials that undergo gelation, the powerlaw relaxation time spectrum, H(tau)~tau^-n for tau,min<tau<tau,max, governs the rheology only in a narrow window very close to the gel point. Soon beyond the gel point, the soft solid develops a very rich

viscoelastic behavior for the evolving material states with increasing connectivity. Typical rheological features of the evolving soft solid are a growing relaxation modulus and accelerated relaxation processes for the structural components that can still relax. Time-resolved rheology measurements, in combination with time-cure superposition, on two model materials show this soft solid behavior. One model material (self-exfoliating clay-polymer composite) represents physical gelation and the other one (crosslinking polyurethane) represents chemical gelation. The relaxation characteristics near the gel point are different for the two materials. For the physically gelling material, the modulus growth was found to be inversely proportional to the relaxation time decay. For chemical gelation, the modulus grows only with a factor of about 0.7. During the next couple of months, more gelling materials are going to be included in the study since it is unclear how widespread the observed viscoelastic pattern occurs.

## CPP 56: Membranes and vesicles II (joint session BP, CPP)

Time: Wednesday 15:00–18:30 Location: H 1028

**Invited Talk** CPP 56.1 Wed 15:00 H 1028

**Caged Hyperpolarized Xenon in Phospholipid Membranes for NMR Sensing Applications** — •Leif Schröder — Leibniz-Institut für Molekulare Pharmakologie (FMP), Berlin, Germany

Spin-hyperpolarized xenon comes with high sensitivity and specificity for NMR spectroscopy due to the large chemical shift range of the dissolved gas. Recent developments in indirect detection of temporarily caged atoms through chemical exchange saturation transfer with hyperpolarized nuclei (Hyper-CEST) allows to sense for the molecular environment of the NMR-active isotope Xe-129 despite being a noble gas. In fact, its tendency to participate in labile van der Waals interactions facilitates very sensitive NMR detection. The hydrophobicity of xenon causes easy partitioning into phospholipid membranes where it can be combined with hydrophobic molecular cages as their hosts that confer a specific chemical shift to the guest nuclei for easy Hyper-CEST detection. The CEST effect is sensitive to exchange dynamics and can therefore be used to characterize the conditions for the specific host-guest system in various environments. This talk will give an overview about applications such as sensing for membrane fluidity and integrity or NMR imaging studies of liposome tracking for targeted drug delivery.

CPP 56.2 Wed 15:30 H 1028

**Lipid composition in fusion of model membrane systems studied by x-ray diffraction** — •Sebastian Köhler[1], Yihui Xu[1], Ziad Khattari[2], and Tim Salditt[1] — [1]Institut für Röntgenphysik, Georg-August-Universität Göttingen — [2]Department of Physics, Hashemite University, Zarqa, Jordan

We have investigated the structure and interaction of solid-supported multilamellar phopholipid bilayers as model systems for membrane fusion in view of the formation of stalks (putative intermediate structures occurring during the fusion process). X-ray reflectivity and grazing incidence small angle x-ray scattering measurements have been performed on bilayer stacks of different ternary and quaternary lipid mixtures at varying osmotic pressure. Analysis of the obtained electron density profiles and pressure-distance curves reveals systematic changes in structure and hydration repulsion. The osmotic pressure needed to induce stalk formation at the transition from the fluid lamellar to the rhombohedral phase indicates how membrane fusion properties are modified by bilayer composition. We present phase diagrams for all studied lipid mixtures.

CPP 56.3 Wed 15:45 H 1028

**VSG dynamics on the Trypanosome and on model membranes** — Marius Glogger[1], Marie Spindler[1], Andreas Hartel[1,2], Nicola Jones[1], Markus Engstler[1], and •Susanne Fenz[1] — [1]Biocenter: Cell and Developmental Biology, University of Würzburg, Würzburg, Germany — [2]Department of Electrical Engineering, Columbia University, New York, New York 10027, United States

Trypanosomes are the pathogens of sleeping sickness in humans and Nagana in cattle. They exhibit a uniform surface coat of multiple copies of variable surface glycoproteins (VSGs). Trypanosomes use this extremely dense, albeit highly dynamic surface coat for protection against the host's innate immune response. The entire VSG surface coat can be exchanged by endocytosis of the old VSG and parallel exocytosis of a new VSG variant within 10 minutes. However, both processes are restricted to a small membrane invagination of the cell surface, the so-called flagellar pocket. The mobility of VSG is essential for the parasite's survival and the focus of our research interest. Trypanosomes are excellent model organisms because 95% of their surface coat consists of VSGs. Thus, comparable measurements in live cells and model membranes will allow us to separate active motion from passive diffusion. As VSGs are abundant they can be easily purified and subsequently integrated into supported lipid bilayers via their membrane anchor. We apply single-molecule fluorescence microscopy to study VSG dynamics in immobilized trypanosomes and model membranes with special emphasis on the modulating character of protein glycosylation.

CPP 56.4 Wed 16:00 H 1028

**Al3+ binding effects on lipid membrane structure** — Hannah Wayment-Steele[1], Sofia Svedhem[2], Lewis E. Johnson[3], Malkiat S. Johal[1], Björn Agnarsson[2], and •Angelika Kunze[4] — [1]Dept. of Chemistry, Pomona College, CA, USA — [2]Dept. of Applied Physics, Chalmers Univ. of Technology, Göteborg, Sweden — [3]Dept. of Chemistry, Univ. of Washington, Seattle, WA, USA — [4]Inst. of Physical Chemistry, Univ. of Göttingen, Göttingen, Germany

Aluminum is found in daily life as a contaminant in food-contact articles as well as in medical and cosmetic products. However, the aluminum ion has been identified as a neurotoxin; several studies have suggested that increased Al3+ concentrations are correlated with increased risks for Alzheimer's disease. The toxicity of the Al3+ derives from structural changes induced in membranes upon binding; it increases membrane rigidity, facilitates vesicle fusion and rupture. However, the mechanisms for these processes are still not fully understood.

Here, we elucidate the effect of Al3+ ions on neutral and charged mixed supported lipid membranes (SLMs) using a variety of surface sensitive experimental techniques in combination with molecular dynamic (MD) simulations.

Our results show that Al3+ affects lipid packing, bilayer thickness, diffusivity as well as it does induce irreversible domain formation in a mixed bilayer. The observed effects for neutral SLMs are mostly reversible whilst the effects observed for mixed SLMs are mostly irreversible. Notably does MD simulations reveal that Al3+ changes the order parameter of the fatty acid chains.

CPP 56.5 Wed 16:15 H 1028

**Ultra-thin self-hydrated artificial membrane composed of DPPC and chitosan deposited without solvents** — Maria J. Retamal[1,2], Marcelo A. Cisternas[1,2], Sebastian E. Gutierrez-Maldonado[3], Tomas Perez-Acle[3], Birger Seifert[1,2], Mark Busch[4], Patrick Huber[4], and •Ulrich G. Volkmann[1,2] — [1]SurfLab UC, Instituto de Fisica, Pontificia Universidad Catolica de Chile (UC), Santiago, Chile — [2]CIEN-UC, Santiago, Chile — [3]DLab, Fundación Ciencia y Vida, Santiago, Chile — [4]Institute of Materials Physics and Technology, Hamburg Univ. of Technology (TUHH), Hamburg-Harburg, Germany

We present the formation and characterization of a phospholipid bilayer (dipalmitoylphosphatidylcholine, DPPC) on a mattress of a polysaccharide (Chitosan) that keeps the membrane hydrated. The deposition of Chitosan (˜25 Å) and DPPC (˜60 Å) was performed from the gas phase in high vacuum onto a substrate of Si(100). The layer thickness was controlled in situ using Very High Resolution Ellipsometry (VHRE). Raman spectroscopy studies show that neither Chitosan nor DPPC molecules decompose during evaporation. With VHRE and AFM we have been able to detect phase transitions in the membrane. The presence of the Chitosan interlayer as a water reservoir is essential for both DPPC bilayer formation and stability. Our experiments at SurfLab UC show that the proposed sample preparation from the gas phase is reproducible and provides a natural environment for the DPPC bilayer. Reference: www.aip.org/publishing/journal-highlights/artificial-membranes-silicon

CPP 56.6 Wed 16:30 H 1028

**Attraction between hydrated hydrophilic surfaces** — •Matej Kanduc[1], Emanuel Schneck[2], and Roland Netz[1] — [1]Department of Physics, Free University Berlin — [2]Max Planck Institute of Colloids and Interfaces, Research Campus Golm

According to common knowledge, hydrophilic surfaces repel via hydration forces while hydrophobic surfaces attract, but mounting experimental evidence suggests that also hydrophilic surfaces can attract. Using all-atom molecular dynamics simulations at prescribed water chemical potential [1] we study the crossover from hydration repulsion to hydrophobic attraction between planar surfaces. We cover the complete spectrum from very hydrophobic surfaces (characterized by contact angles of 135°) to hydrophilic surfaces exhibiting complete wetting. Indeed, for a finite range of contact angles between 65° and 90°, we find a regime where hydrophilic surfaces attract at subnanometer separation and stably adhere without intervening water, in good agreement with experiments. Analysis of the total number of hydrogen bonds (HBs) formed by water and surface groups rationalizes this crossover between hydration repulsion and hydrophilic attraction in terms of a subtle balance [2]. Such solvent reorganization forces presumably underlie also other important phenomena, such as selective ion adsorption to interfaces as well as ion pair formation.

[1] M. Kanduc, A. Schlaich, E. Schneck, and R. Netz; Adv. Colloid Interface Sci. 208, 142 (2014).

[2] M. Kanduc, E. Schneck, and R. Netz; Chem. Phys. Lett. 610, 375-380 (2014)

**15 min break**

CPP 56.7 Wed 17:00 H 1028

**Vesicles-on-a-chip: versatile fabrication of liposomes and polymersomes in microfluidic environment** — •Julien Petit, Ingmar Polenz, Stephan Herminghaus, and Oliver Bäumchen — Max Planck Institute for Dynamics and Self-Organization (MPI-DS), 37077 Göttingen, Germany

Synthetic biology recently appeared as an emerging field of research for mimicking and understanding natural systems from a fundamental point of view. This "bottom-up" approach involves the investigation of the biological and physical properties and mechanisms of functional biological systems (from basic modules/parts of living cells to more complicated systems). One key challenge relies on the fabrication of compartments such as vesicles, that can be viewed as model membranes, as demonstrated by numerous studies during the past decades. Despite this fact, reliable methods for high-throughput production of vesicles (liposomes as well as polymersomes) in an easy and well-controlled manner are still in progress. In this scope, we propose a versatile method for producing monodisperse vesicles in a microfluidic environment from double-emulsions templates. The combination of the microfluidic chip design and the original channel treatment as well as the new fluid systems employed in the present study allows the production and manipulation of liposomes and polymersomes on demand. This new technique opens a playground for fundamental studies, e.g. on the collective behavior of vesicle clusters and their self-organization, as well as applications such as protein or drug encapsulation and mechanisms of targeted delivery.

CPP 56.8 Wed 17:15 H 1028

**High resoultion mapping of the surface charge density of lipid bilayers under physiological conditions** — •Thomas Fuhs, Lasse Hyldgaard Klausen, Flemming Besenbacher, and Mingdong Dong — Interdisciplinary Nanoscience Center (iNANO), Aarhus University, Aarhus, Denmark

The surface charge density of lipid bilayers governs the cellular uptake of charged particles and guides cell-cell and cell-surface interactions. Direct probing of the potential requires sub nanometer distances as the electrostatic potential is screened by high physiological salt concentrations. This prevented direct measurement of the SCD under physiological conditions. In this study we investigate supported bilayers of lipid mixtures that form domains of distinct surface charges, submerged in 150mM NaCl. We use a scanning ion-conductance microscope (SICM) setup to measure the ionic current through a nanopipette as the pipette is scanned several nm above the sample. The charged headgroups of the lipids attract counter ions leading to a charge dependent enhancement of the ion concentration near the surface. This creates a measurable change of conductivity in the vicinity of the surface. As the dependency of the current on the SCD and pipette potential is nontrivial we characterized it using numerical solutions to Poisson and Nernst-Planck equations. Based on the simulation results we propose an imaging method. We confirm feasibility of the proposed method by experimentally mapping the local surface charge density of phase separated lipid bilayers.

CPP 56.9 Wed 17:30 H 1028

**From destruction to protection - following peptide interactions with membrane interfaces** — •Johannes Franz[1], Denise Schach[1], Joe E. Baio[2], Dan Graham[3], David G. Castner[3], Mischa Bonn[1], and Tobias Weidner[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Oregon State University, Corvallis, OR, USA — [3]University of Washington, Seattle, WA, USA

The cell membrane is the most important biological surface as its interaction with peptides is an integral part of transport, communication, energy transduction and survivability. However, an intrinsic difficulty in monitoring peptide interaction with membranes is the required surface sensitivity. Sum frequency generation (SFG) vibrational spectroscopy is well suited to study protein monolayers at lipid surfaces because of its inherent surface specificity. In this study, two different peptides are shown to interact with model membranes in very different ways.

GALA, a peptide mimicking viral fusion proteins, can disrupt membranes and escape from endosomes when triggered at low pH. We follow GALA activity at the molecular level and probe peptide folding as well as the disturbance and hydration of individual leaflets within model bilayers. We show that the cell-penetrating peptide SAP(E) solely interacts with the lipid headgroup region proving the first step of its proposed uptake mechanism. Peptides can also help stabilize lipid membranes. We discuss preliminary results about the effects of specific antifreeze proteins on the temperature stability of lipid mono- and bilayers.

CPP 56.10 Wed 17:45 H 1028

**Addressing Multivalent Interactions Using Single Particle Tracking** — •Stephan Block, Srdjan Acimovic, Mikael Käll, and Fredrik Höök — Department of Applied Physics, Chalmers University of Technology, Gothenburg, Sweden

Multivalent interactions are observed in a multitude of biological processes (e.g., association of viruses or bacteria to their host cells). The involved receptors are nano-sized objects, making it challenging to assess the exact number of attachment points under physiological conditions. Using TIRF microscopy of fluorescently labelled, small unilamellar vesicles, which serve as a model system for the interaction of viruses with cell membranes, we show that multivalent interactions can be assessed by single particles tracking (SPT). The vesicles are linked to a supported lipid bilayer (SLB) using DNA-tethers carrying cholesterol groups at their ends, which automatically insert into the membranes and which allow a 2D diffusion of the vesicle above the SLB. The number of attachment points can be manipulated by the concentration ratio of vesicles to DNA-tethers. SPT allows to extract the diffusion coefficients on the level of single vesicles and histograms of the observed diffusion coefficients exhibit a spectrum of distinct peaks, which are related to subpopulations of vesicles differing by their number of DNA-tethers. This enables to recalculate fluctuations of the diffusion constant of a certain vesicle into fluctuations of the number of attachment points linking the vesicle to the SLB. The extension of this analysis to virus particle tracking including a comparison between SPT with fluorescence correlation spectroscopy will be discussed.

CPP 56.11 Wed 18:00 H 1028

**Fast tracking with nanometer precision of individual proteins on the cell membrane** — •Richard Taylor and Vahid Sandoghdar — Max Planck Institute for the Science of Light, Erlangen, Germany

The diffusion dynamics of membrane-incorporated proteins in the live cell is of great biological significance, but its studies are complicated and nuanced due to the diversity and heterogeneity of the membrane landscape. While fluorescence microscopy is routinely employed to investigate membrane phenomena, a low fluorescence rate and photobleaching limit this technique both on the short and long time scales. Furthermore, fluorescence microscopy suffers from a poor axial resolution.

Here, we report on the use of interferometric scattering (iSCAT) imaging with high three-dimensional spatio-temporal resolution. By labelling the proteins with a small gold nanoparticle, we are able to track indefinitely the protein diffusion in and out of plane, to an unparalleled nm-level accuracy at many thousands of frames per second. We present recent work on tracking of EGFR proteins in the model HeLa cell. Furthermore, we discuss the use of iSCAT imaging for studying out-of-membrane movement, thus allowing investigation into endocytotic reactions.

CPP 56.12 Wed 18:15 H 1028

**The interaction of patterned amphiphilic dendritic nanomaterial with a lipid-monolayer** — •M.Alejandra Sanchez, Katharina Bücher, Klaus Müllen, Mischa Bonn, and Ellen H.G Backus — Max Planck Institute for Polymer Research, Mainz, Germany

Well-defined amphiphilic dendrimeric macromolecules are biomimetic nanomaterials that can be used for drug delivery into cells. By organic synthesis, functional groups can be positioned in an atomically defined way, resulting in alternating patches of polar and apolar nature. Here we study systematically the interaction of various dendrimers with a model membrane consisting of a self-assembled monolayer of the lipid DPPC (1,2-dipalmitoyl-sn-glycero-3-phosphocholine) on water. By using sum frequency generation spectroscopy we obtain molecular specific information about the membrane molecules and the water molecules in the vicinity of the lipid. Although the dendrimers are not surface-active at the bare water-air interface, they do interact strongly with the lipid monolayer. The presence of dendrimers in the solution below the monolayer causes changes in the water orientation as well as the alignment of the lipid molecules. Remarkably, details of the interaction depend on the surface groups present on the dendrimer. Very small changes (e.g. n-propyl vs iso-propyl) result in a different behavior. We link the molecular level picture with the efficiency of penetrating into the cells.

## CPP 57: Complex Fluids and Soft Matter - Part I (joint session DY, CPP, BP)

Time: Wednesday 15:00–16:45 Location: BH-N 333

CPP 57.1 Wed 15:00 BH-N 333

**Particle segregation in a sedimenting bidisperse soft sphere system** — Matthias Kohl and •Michael Schmiedeberg — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40204 Düsseldorf, Germany

We explore the sedimentation process of a binary soft colloidal sphere system. In case of large overlaps of the particles the segregation dynamics differs significantly from that of hard particles. By using Brownian dynamics simulations and theoretical predictions, we find new complex states [1]. For example, multiple-phase-stackings where large particles gather both at the top and the bottom of the system or metastable network-like structures occur. We analyze the comprehensive dynamics of the segregation process. Usually, we observe a multiple-step process: First there is local segregation, then clusters are formed, and finally the clusters sink to their equilibrium position.

[1] M. Kohl and M. Schmiedeberg, Soft Matter 10, 4340 (2014).

CPP 57.2 Wed 15:15 BH-N 333

**Suppression of Ostwald Ripening by Chemical Reactions in Active Emulsions** — •David Zwicker[1,2], Anthony A. Hyman[3], and Frank Jülicher[2] — [1]Harvard University, Cambridge MA, USA — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Max Planck Institute of Cell Biology and Genetics, Dresden, Germany

Ostwald ripening is a coarsening process of droplets in an emulsions that is driven by the surface tension of the droplets. This coarsening must be suppressed to stabilize emulsions, e.g. to control the properties of pharmaceuticals, food, or cosmetics. Ostwald ripening must also be suppressed in biological cells, which contain liquid-like compartments, e.g. germ granules, Cajal-bodies, and centrosomes. Such systems are often driven away from equilibrium by chemical reactions and can thus be described as active emulsions.

Here, we show that non-equilibrium chemical reactions can suppress Ostwald Ripening, leading to stable, monodisperse emulsions. Using a coarse-grained description of the droplet dynamics, we derive analytical approximations of the typical droplet size, droplet count, and time scale of the dynamics. We also compare these results to numerical simulations of the continuous concentration fields. We thus show how chemical reactions can be used to stabilize emulsions and control their properties.

CPP 57.3 Wed 15:30 BH-N 333

**Binary mixtures of hard rod–like colloids: mesoscopic equilibrium theory and shear-driven instabilities** — •Rodrigo Lugo Frias and Sabine Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Mixtures of rod–like particles occur in a wide range of biological contexts and technological applications, and their equilibrium phase behavior has been intensely studied in recent years. Here we investigate a binary mixture of rod–like colloidal particles driven out of equilibrium by means of a steady shear flow (Couette geometry).

Using classical density functional theory (DFT), we first derive a mesoscopic free energy functional for a mixture of hard spherocylinders with different length–to–length ratio in terms of tensorial order parameters that describe their alignment. The resulting free energy displays a strong dependence on the microscopical properties of the system. Based on the equilibrium analysis, we then discuss the dynamical behavior of the mixture using a natural extension of the mesoscopic Doi–Hess theory. In particular we analyze the orientational dynamics under shear for varying shear rate, concentration and aspect ratio.

[1] F. Tardani, L. Gentile, G. A. Ranieri and C. La Mesa, J. Phys. Chem. C, **117**, 8556 (2013).

[2] S. Hess, Z.Naturforsch. A **31a**, 1034 (1976). M. Doi, J.Polym. Sci., Polym. Phys. Ed. **19**, 229 (1981).

[3] R. Lugo-Frias and S. H. L. Klapp, in preparation (2015).

CPP 57.4 Wed 15:45 BH-N 333

**Dynamics of the Critical Casimir Effect in a Binary Fluid** — •Sutapa Roy, Felix Höfling, and S. Dietrich — Max-Planck-Institut für Intelligente Systeme, Stuttgart and Institut für Theoretische Physik IV, Universität Stuttgart, Germany

A binary fluid mixture near its consolute point exhibits critical fluctuations of the local composition. While the static properties of the mixture are well described by the 3D Ising universality class [1], the dynamic properties involving conservation of particle number and concentration, energy, and momentum are classified as model $H'$ [2]. Confinement of critical fluctuations in such a mixture leads to critical Casimir forces (CCF) [3] acting on the confining surfaces.

We present results for the CCF in a symmetric binary Lennard-Jones model fluid, confined in a slit pore, close to its bulk critical point. Utilizing the computing resources of GPUs [4], molecular dynamics (MD) simulations were performed for system sizes of up to 216,000 particles and 5 orders of magnitude in time which is well beyond common computational efforts. Our results from MD and Monte Carlo simulations, for various static and dynamic quantities, both in bulk and in confinement, are compared to theory and experimental observations.

[1] S.K. Das *et al.*, J. Chem. Phys. **125**, 024506 (2006).

[2] P.C. Hohenberg and B.I. Halperin, Rev. Mod. Phys. **49**, 435 (1977).

[3] C. Hertlein, L. Helden, A. Gambassi, S. Dietrich and C. Bechinger, Nature **451**, 172 (2008).

[4] P. Colberg and F. Höfling, Comput. Phys. Commun. **182**, 1120 (2011).

CPP 57.5 Wed 16:00 BH-N 333

**Simulating many-body Casimir interactions in colloidal suspensions** — •Hendrik Hobrecht and Fred Hucht — Fakultät für Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg

We study the fluctuation-induced (Casimir) interactions in colloidal suspensions, especially between colloids immersed in a binary liquid close to its critical demixing point for two-dimensional systems. To simulate those systems, we present a Monte Carlo cluster algorithm based on geometric symmetries of the Hamiltonian. Utilizing the principle of universality, the suspension is represented by an Ising system while the colloids are areas of spins with fixed orientation. Our results for the Casimir interaction potential between two particles agree quantitatively with the theoretical predictions [1], where we find that the behavior depends strongly on whether the order parameter is hold fixed or is allowed to fluctuate. Finally we present our results for the three-body interaction Casimir potential.

[1] T. W. Burkhardt and E. Eisenriegler, Phys. Rev. Lett. 74 (1995) 3189.

CPP 57.6 Wed 16:15 BH-N 333

**Flow induced deflection of a liquid-crystal topological defect** — Tillmann Stieger[1], Martin Schoen[1], and •Marco G. Mazza[2] — [1]Technische Universität Berlin — [2]Max-Planck-Institut für Dynamik und Selbstorganisation

We perform nonequilibrium molecular dynamics simulations of a nematic liquid crystal flowing around a colloidal particle. We study the flow-induced modifications of the Saturn ring defect and the surface ring defect in the liquid crystal. By varying the strength of the interaction between liquid crystal and colloid we can produce Saturn rings of different sizes. We study the deflection of the topological defect as a function of applied stress, and find a linear, that is Hookean, stress-strain dependence. We relate this finding to the elastic properties of the nematic liquid crystal and to the properties of the core of the topological defect.

CPP 57.7 Wed 16:30 BH-N 333

**Modeling drying droplets on porous substrates** — •Christian Diddens[1], Hans Kuerten[1], Cees van der Geld[1], and Herman Wijshoff[1,2] — [1]Eindhoven University of Technology, The Netherlands — [2]Océ Technologies B.V., Venlo, The Netherlands

We investigate the drying of an inkjet-printed picoliter droplet on a porous substrate in the framework of a numerical model. The evolution of the droplet is governed by evaporation at the liquid-air interface and absorption of the liquid into the porous substrate.

When a binary mixture is considered, an interplay of preferential evaporation, composition-dependent viscosity and the absorption dynamics can interestingly result in a slower drying for faster evaporation rates.

Since solute particles and their deposition to the surface are also taken into account, the present model can be utilized as predictive tool for deposition patterns in ink-jet printing processes.

## CPP 58: Computational Physics of Soft Matter II

Time: Wednesday 15:45–18:30 Location: PC 203

**Invited Talk** CPP 58.1 Wed 15:45 PC 203

**The Tricontinuous 3ths(5) Phase: A New Morphology in Copolymer Melts** — •Gerd Schroeder-Turk[1,2,3], Michael Fischer[1,2,4], Liliana de Campo[2,5], Jacob Kirkensgaard[6], and Stephen Hyde[2] — [1]Theor. Physik, Fried.-Alex. Univ. Erlangen-Nürnberg, Germany — [2]Applied Maths, Res. School of Physics & Eng., Australian National Univ., Canberra, Australia — [3]School of Engineering & Inform. Technol., Murdoch Univ., Western Australia — [4]Adolphe Merkle Institute, Fribourg, Switzerland — [5]Australian National Science & Technol. Organisation, Bragg Institute, NSW, Australia — [6]Niels Bohr Institute, Univ. of Copenhagen, Denmark

Self-assembly remains the most efficient route to the formation of ordered nanostructures, including the double gyroid network phase in diblock copolymers based on two intergrown network domains. Here we use self-consistent field theory to show that a tricontinuous structure with monoclinic symmetry, called 3ths(5), based on the intergrowth of three distorted ths nets, is an equilibrium phase of triblock star-copolymer melts when an extended molecular core is introduced. The introduction of the core enhances the role of chain stretching by enforcing larger structural length scales, thus destabilizing the hexagonal columnar phase in favor of morphologies with less packing frustration. This study further demonstrates that the introduction of molecular cores is a general concept for tuning the relative importance of entropic and enthalpic free energy contributions, hence providing a tool to stabilize an extended repertoire of nanostructured phases.
Reference: Fischer *et al*, Macromolecules **47**, 7424-7430 (2014)

CPP 58.2 Wed 16:15 PC 203

**Coarse-grained electrostatic interactions for symmetric disk-shaped molecules** — •Thomas Heinemann[1], Karol Palczynski[2], Joachim Dzubiella[2], and Sabine H. L. Klapp[1] — [1]Institut für Theoretische Physik, TU Berlin, 10623 Berlin — [2]Institut für Physik - Komplexe Systeme, HU Berlin, Newtonstr. 15, 12489 Berlin

In the present study we introduce a novel route for calculating temperature-dependent effective pair potentials of disk-shaped molecules with van der Waals and electrostatic interactions. An ideal candidate for this study is the coronene molecule. For this molecule, an anisotropic and temperature-dependent coarse-grained model describing van der Waals interactions already exists [1]. Here we extend the approach towards electrostatic interactions. The electrostatic potential can be described through a set of differently charged rings [2]. However, the evaluation of the intermolecular ring-ring interactions is numerically quite involved. Therefore we introduce two strategies to cope with the ring–ring interactions. The first strategy aims at representing the entire electrostatics, given by the concentric set of rings, through a linear point quadrupole. In the second strategy, we fit the combined potential consisting of van der Waals and ring-ring-contributions with an extended van der Waals model. We discuss the applicability of both models and compare many-particle simulation results for crystalline structures with experimental data.

[1] T. Heinemann, K. Palczynski, J. Dzubiella and S. H. L. Klapp, J. Chem. Phys., in press, arXiv: 1407.4352

[2] Obolensky et al., Int. J. Quantum Chem. 107, 1335 (2007).

CPP 58.3 Wed 16:30 PC 203

**Brownian Dynamics simulations on soft patchy particles made of isotropic spheres** — •Malte Lütje — Universität Tübingen

Patchy Particles are widely used as a model system for proteins in a solution. We propose a dynamical model for patchy colloidal particles emerging from a binary mixture of particles of different size, "colloids" and "bonds". Both colloids and bonds interact with isotropic, but non-additive hard-sphere interactions, additionally the colloid-bond interaction contains a short-range, isotropic attraction. Our model resembles a soft version of the model studied by E. Zaccarelli et al. [1]

Equilibrium and dynamical properties of the mixture are investigated by Brownian Dynamics simulations. Due to the repulsion among the bonds a finite number of binding sites on a colloid is achieved.

We focus on a maximum number of four binding sites on each colloid, rendering possible a tetrahedral structure. Upon varying bond concentration, temperature and packing fraction $\phi$ of the colloids, we equilibrate the system and examine the resulting structures. Of particular interest is the transition from a locally clustered state at small volume fractions of colloids to the emerging tetrahedral network that was found in Ref. [1] for $\phi \geq 0.22$.

[1] E. Zaccarelli, F. Sciortino, P. Tartaglia, J. Chem. Phys. 127, 174501 (2007)

CPP 58.4 Wed 16:45 PC 203

**Self organization of asymmetric dipolar particles in external fields** — •Arzu Bahar Yener and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

A colloidal system of spherical particles with centred dipolar moments shows layer formation in the presence of an external rotating magnetic field [1]. This non-equilibrium phenomenon requires synchronization of the particles with the driving field [1]. Here, we investigate a model system of spherical particles with off-centred, i.e. laterally shifted dipole moments. The pair potential is modeled by a short-range repulsive potential and a point dipole potential. In a first step, we analytically and numerically determine the ground state structures of up to four particles. Then, we quantify the self assembly behaviour at non-zero temperature for several shifts by using Molecular Dynamics simulations and show that our model reproduces features observed for synthesized particles with magnetic caps [2] or Janus particles [3]. Finally, we apply an external rotating magnetic field and ask if layer formation emerges as in the centred system, and if synchronization is still a condition for layer formation.
[1] S. Jäger, and S. H. L. Klapp, Soft Matter **7**, 6606 (2011)

[2] D. Zerrouki, J. Baudry, D. Pine, P. Chaikin, and J. Bibette, Nature **455**, 380 (2008)
[3] J. Yan, M. Bloom, S. C. Bae, E. Luijten, and S. Granick, Nature **491**, 578 (2012)

CPP 58.5 Wed 17:00 PC 203

**Assessing the Quality of Ab Initio Molecular Dynamics Simulations of Water by High-Dimensional Neural Network Potentials** — Tobias Morawietz[1], Andreas Singraber[2], Christoph Dellago[2], and •Jörg Behler[1] — [1]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Computational Physics, Universität Wien, Sensengasse 8/9, A-1090 Vienna, Austria

Ab initio molecular dynamics simulations have become a standard tool to study the properties of water, but they are severely hampered by the computational costs if long simulations of large systems are required. In recent years, interatomic potentials based on artificial neural networks (NNs) have been shown to provide very efficient and accurate potential-energy surfaces close to the reliability of electronic structure methods. Here we present a set of NN potentials for water based on density-functional theory. We demonstrate that these potentials can be used to assess the quality of different exchange-correlation functionals and the importance of van der Waals interactions in the description of liquid water.

CPP 58.6 Wed 17:15 PC 203

**Proton disorder in cubic ice: Effect on the electronic and optical properties** — Viviana Garbuio[1], Olivia Pulci[1], Michele Cascella[2], Igor Kupchak[3], and •Ari Paavo Seitsonen[4,5] — [1]MIFP, ETSF, Dipartimento di Fisica, Università di Roma Tor Vergata, Italy — [2]Department of Chemistry and Centre for Theoretical and Computational Chemistry, University of Oslo, Norway — [3]MIFP, V. Lashkarev Institute of Semiconductor Physics of National Academy of Sciences of Ukraine, Kiev — [4]Institut für Chemie, Universität Zürich, Switzerland — [5]Département de Chimie, École Normale Supérieure, Paris, France

The proton disorder in ice has a key role in several properties such as the growth mode, thermo- dynamical properties and ferroelectricity. While structural phase transitions from proton disordered to proton ordered ices have been extensively studied, much less is known about their electronic and optical properties. Here, we present ab-initio many body perturbation theory based calculations of the electronic and optical properties of cubic ice at different levels of proton disorder. We compare our results with liquid water, as an example of fully (proton and oxygen) disordered system. We find that, by increasing the disorder, a shrinking of the electronic gap occurs. Simultaneously, the excitonic binding energy decreases, so that the final optical gaps result to be almost independent on the degree of disorder. We explain these findings as an interplay between the local dipolar disorder and the electronic correlation.

CPP 58.7 Wed 17:30 PC 203

**Molecular dynamics simulation of the dielectric permittivity tensor at the water/1,2-dichloroethane liquid-liquid interface** — •Zhu Liu, Hendrik H. Heenen, Karsten Reuter, and Christoph Scheurer — Technische Universität München

The liquid-liquid Interface between Two Immiscible Electrolyte Solutions (ITIES) has been the focus of scientific interest for decades [1,2]. One important continuum response property of the liquids at the interface is expressed by the dielectric permittivity tensor, which sensitively reflects the unique microscopic characteristics in the interfacial region. The dielectric permittivity is known to change across the liquid-liquid interface, varying between the isotropic values for the pure liquids in the limit of the bulk far away from the interface. Recent work by Netz *et al.* based on Molecular Dynamics (MD) simulations for water at a solid-liquid interface revealed a rather unexpected behavior of the dielectric permittivity tensor as a function of the distance from the interface [3]. To our knowledge no comparable investigations are currently available for liquid-liquid interfaces. We present results for the prototypical water/1,2-dichloroethane (DCE) liquid-liquid interface making use of our recent implementation of a suitable polarizable force field in the Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS).

[1] A.G. Volkov *et al.*, Liquid-Liquid Interfaces: Theory and Methods, CRC Press, New York (1996).
[2] Z. Samec, Electrochimica Acta **84**, 21 (2012).
[3] D.J. Bonthuis *et al.*, Langmuir **28**, 7679 (2012).

CPP 58.8 Wed 17:45 PC 203

**Quantum-Classical Adaptive Coupling in Grand-Canonical like Adaptive Resolution Simulations** — •Animesh Agarwal and Luigi Delle Site — Institute for Mathematics, Arnimallee 6, D-14195, Freie Universität, Berlin, Germany

We have extended the recently developed Grand Canonical AdResS (GC-AdResS)[1, 2] to quantum-classical adaptive coupling where the quantum delocalisation of an atom is described by the path integral formalism. Compared to standard adaptive coupling approaches [3], the advantage of GC-AdResS is that there is no need to obtain a coarse-grained model that correctly reproduces the structural and thermodynamic properties of a full PI (path integral) system, thereby eliminating the need to run a full PI simulation before starting the adaptive simulation. In this context, we have shown that spherical molecules described by a simple generic WCA potential in the coase-grained region, act as a particle reservoir for the PI region. The resulting Grand Canonical set up is such that the structural and dynamical properties of quantum flexible water models in the PI subregion in AdResS are consistent with the properties obtained in the same subregion in full PI simulations.

[1] H.Wang, C.Hartmann, C.Schütte and L.Delle Site, Phys.Rev.X **3**, 011018 (2013)
[2] A.Agarwal, H.Wang, C.Schütte and L.Delle Site,J.Chem.Phys. **141**, 034102 (2014)
[3] A.B. Poma and L.Delle Site, Phys. Rev. Lett. **104**, 250201 (2010)

CPP 58.9 Wed 18:00 PC 203

**Reactive molecular dynamics simulation of the twin polymerization process with ReaxFF** — Thomas Schönfelder[1], •Janett Prehl[1], Joachim Friedrich[2], Steffen Seeger[1], Stefan Spange[3], and Karl Heinz Hoffmann[1] — [1]Computerphysik, Technische Universität Chemnitz — [2]Theoretische Chemie, Technische Universität Chemnitz — [3]Polymerchemie, Technische Universität 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. To gain insights into formation processes we implement a first-principles-based ReaxFF reactive force field for C/H/O/Si for the initial electrophilic substitution of an aromatic system [1]. In this presentation we first give a brief introduction to the details of twin polymerization and afterward we present our progress [2] in establishing an appropriate reactive force field parametrization to model all partial reaction steps and the subsequent polymerization at least for small system sizes.

[1] T. Schönfelder, J. Friedrich, J. Prehl, S. Seeger, S. Spange, and K. H. Hoffmann, *Chem. Phys.* **440** (2014) 119-126
[2] T. Schönfelder, J. Prehl, J. Friedrich, and K. H. Hoffmann, to be submitted

CPP 58.10 Wed 18:15 PC 203

**Development of the extended ReaxFF+ approach to accurately model ionic system** — •Oliver Böhm, Stephan Pfadenhauer, and Philipp Plänitz — AQcomputare GmbH, 09125 Chemnitz, Germany

In order to be able to describe ionic systems within a liquid environment we have extended the original bond order dependend reactive force field (ReaxFF) of the van Duin group [1]. The new approach is called ReaxFF+ [2]. It uses a new charge equilibrium scheme which is able to model ionic as well as neutral systems. The main goal is the correct description of the ionic and and covalent behaviour of bonds. This is realized by a bond order dependent Coloumb screening and an electronegativity which is a function of the over- and undercoordination. This allows the simulation of reactions in basic and acid solutions as well as the charge transfer in bond breaking reactions of neutral molecules. The accuracy of the scheme is demonstrated for different ionic molecules.

[1] A. van Duin et al., J. Phys. Chem. A, 105, 9396 (2001); J. Phys. Chem. A, 107, 3803 (2003)
[2] O. Böhm et al., J. Am. Chem. Soc. (2015) submitted

## CPP 59: CPP Mitgliederversammlung

Mitgliederversammlung des Fachverbandes Chemische Physik und Polymerphysik. Im Rahmen der Mitgliederversammlung findet die Verleihung des Posterpreises, gestiftet von Asylum Research, satt. Im Anschluss gemütliches Beisammensein mit Imbiss und Getränken.

Time: Wednesday 18:30–19:30 Location: C 130

**60 minutes meeting**

## CPP 60: Focus Session Hybrid Photovoltaics and Prevovskites I (joint session CPP HL, O)

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

**Invited Talk** CPP 60.1 Thu 9:30 C 130

**Advances in hybrid solar cells: From hybrid organic/inorganic to perovskite photovoltaics** — •Lukas Schmidt-Mende — University of Konstanz

In this presentation we will discuss the path from solid-state dye sensitized solar cells over extremely thin absorber cells towards perovskite solar cells. Hybrid solar cells have been investigated for some time and a lot of knowledge gained in this field has helped to increase the power conversion efficiencies of recently discovered perovskite solar cells from 2.2% when first reported in 2006 to over 20% in 2014. Going from liquid electrolyte cells to solid-state hybrid solar cell architecture had a major influence on this performance step. Many structures previously used in hybrid solar cells have been now implemented very successfully in perovskite solar cells. We will give some examples of such knowledge transfer from conventional hybrid solar cells to perovskite solar cells. A discussion of the similarities as well as the differences of the described solar cell types will help to understand possible limitations.

CPP 60.2 Thu 10:00 C 130

**Electron tomography of interpenetrating polymer:nanocrystal networks as photoactive layers in hybrid solar cells: correlations between the morphology and device performance** — •Holger Borchert, Christopher Krause, Dorothea Scheunemann, and Jürgen Parisi — Carl von Ossietzky University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, 26111 Oldenburg, Germany

Hybrid bulk heterojunction solar cells use as absorber layer an interpenetrating network of conductive polymer and inorganic semiconductor nanocrystals. Thereby, the nanomorphology of the blend layers plays an important role for the functionality of the devices. On the one hand, the absorber layer should have a large interface between both material components in order to enable efficient separation of electron-hole pairs. On the other hand, continuous pathways for electrons through the nanoparticle phase and holes through the polymer phase are required in order to enable efficient transport of the charge carriers towards the electrodes. A unique technique to investigate the three-dimensional morphology of such hybrid material layers is electron tomography, where three-dimensional images are reconstructed from a series of transmission electron micrographs recorded under different angles. In the present contribution, we investigated active layers consisting of poly(3-hexylthiophene) and colloidally prepared copper indium disulfide nanocrystals. Correlations between the morphology of the blend layers and the electrical performance of hybrid solar cells are analyzed in dependence of varied preparation parameters.

CPP 60.3 Thu 10:15 C 130

**Laser-ablated titania nanoparticles for aqueous processed hybrid solar cells** — •Volker Körstgens[1], Stephan Pröller[2], Christoph Mayr[1], Gonzalo Santoro[3], Stephan V. Roth[3], Hristo Iglev[4], Reinhard Kienberger[4], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85848 Garching — [2]TU München, Munich School of Engineering, James-Franck-Str. 1, 85748 Garching — [3]DESY Photon Science, Notkestr. 85, 22607 Hamburg — [4]TU München, Physik-Department, LS Laser- und Röntgenphysik, James-Franck-Str. 1, 85748 Garching

Hybrid solar cells are produced by applying a new water-based processing method. The active layer consists of titanium dioxide nanoparticles produced by laser ablation in liquid and the water-soluble hole-conducting polymer poly[3-(potassium-6-hexanoate)thiophene-2,5-diyl] (P3P6T). The production of $TiO_2$ nanoparticles via laser ablation in liquid is tested with two approaches, using $TiO_2$ powder as target and a solid titanium target. The crystallinity of both components of the active layer, laser-ablated $TiO_2$ and P3P6T is investigated with X-ray diffraction (XRD) and grazing incidence wide angle X-ray scattering (GIWAXS). A key factor for the performance of the active layer is the functionalization of $TiO_2$ with the polymer P3P6T, which is probed with spectroscopic methods. The hybrid solar cells show high fill factors and open circuit voltages underlining the potential of the novel material and the environment-friendly processing method.

CPP 60.4 Thu 10:30 C 130

**Junction formation and current transport mechanisms in hybrid n-Si/PEDOT:PSS solar cells** — •Sara Jäckle[1], Matthias Mattiza[2], Manuela Göbelt[1], and Silke Christiansen[1,2] — [1]Max-Planck-Institute for the Science of Light, Erlangen, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Hybrid photovoltaics combining a transparent highly conductive polymer and an absorbing inorganic semiconductor promise efficient charge carrier separation and transport. We present solar cells with the 'metal'-like wide-gap polymer PEDOT:PSS and n-doped silicon archiving an open-circuit voltages up to 640mV and a power conversion efficiencies of 12%. The hybrid charge separating interface is commonly treated as a majority carrier dominated Schottky junction. Capacity- and current-voltage characteristics proof by investigating n-Si/PEDOT:PSS solar cells with varying silicon substrate doping concentrations that an inversion layer is created on the silicon surface and the charge transport is dominated by minority carriers. We will present a hybrid junction schematic explaining the promising solar cell characteristics. Furthermore possible degradation mechanisms of these hybrid solar cells under ambient conditions and the effect of encapsulation with low temperature deposited metal oxides will be discussed.

CPP 60.5 Thu 10:45 C 130

**A Comparative Study of Polythiophene/c-Si Hybrid Solar Cells and Inorganic a-Si:H/c-Si Devices** — •M. Zellmeier[1], T. Brenner[2], S. Janietz[3], N. H. Nickel[1], and J. Rappich[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium Photovoltaik, Kekulèstr. 5, 12489 Berlin — [2]University of Potsdam, Institute of Physics & Astronomy, Karl-Liebknecht-Straße 24-25, 14476 Potsdam-Golm — [3]Fraunhofer-Institut für Angewandte Polymerforschung (IAP), Abteilung Polymere und Elektronik, Geiselbergstr. 9, 14476 Potsdam

Non-excitonic polymer/silicon heterojunction solar cells regularly exceed power conversion efficiencies (PCE) of 10%. In combination with the possibility to use solution processing to form an electron-hole separating junction, this device type becomes highly attractive due to its potential for low cost processing. Here, we present a study in which P3HT/c-Si hybrid devices are compared to a-Si:H/c-Si heterojunctions. The advantages of the narrow absorption band of P3HT are pointed out using quantum efficiency measurements. Furthermore, the influence of the intrinsic interlayer (SiOx, Methylgroups) in the final device is investigated and directly compared to equivalent structures (SiOx, intrinsic a-Si:H) in the inorganic devices. The wafer lifetime with and without polymer was examined using quasi steady state photoconductance measurements (QSSPC) and interpreted regarding their influence on the open circuit voltage. The obtained results were used to improve the hybrid devices, leading to a high-performance hybrid solar cell with an open circuit voltage of 659 mV and a PCE of 11%.

CPP 60.6 Thu 11:00 C 130

**High efficiency hybrid triple junction solar cells comprising of amorphous silicon and low band gap polymers exceeding 11 % Power Conversion Efficiency.** — •Steffen Roland[1], Sebastian Neubert[2], Steve Albrecht[1], Bernd Stannowski[2], Mark Seger[3], Antonio Facchetti[3], Rutger Schlatmann[2], Bernd Rech[2], and Dieter Neher[1] — [1]University of Potsdam, Institute of Physics and Astronomie, Potsdam, Germany — [2]PVcomB/Helmholtz-Zentrum Berlin für Materialien und Energie GmBh, Berlin, Germany — [3]Polyera Corporation, Illinois, USA

Merging inorganic and organic solar cells in a series connected hybrid multi-junction is shown to be an elegant approach to prepare efficient solar cells with a total active layer thickness well below 1 $\mu$m. Complementary absorption, high absorption coefficients, and the ease of fabrication make organic low band-gap (LBG) materials, mixed with PC$_{61}$BM, suitable for the use in multi-junction solar cells in combination with amorphous silicon (a-Si:H). Transfer matrix based optical modeling was employed to predict the optimum layer thicknesses of each. External quantum efficiency measurements show that all planar hybrid multi-junctions are current limited by the a-Si:H middle junction. Light scattering front contacts are used to increase the absorption and thereby currents in the amorphous silicon sub-cells. The presented multi-junction solar cells are highly efficient, showing high open circuit voltages and high fill factors up to 80 %. Therefore, merging inorganic/organic sub-cells in multi-junction devices bears great potential as efficient, truly thin film solar cells.

**15 min. break.**

**Invited Talk** CPP 60.7 Thu 11:30 C 130

**The solid state physics of hybrid perovskites** — •Jarvist Moore Frost[1], Federico Brivio[1], Keith Butler[1], Aurelien Leguy[2], Artem Bakulin[3], Piers Barnes[2], and Aron Walsh[1] — [1]University of Bath, Bath, United Kingdom — [2]Imperial College London, London, United Kingdom — [3]Cambridge University, United Kingdom

Hybrid perovskites offer rich solid state physics. Here we apply electronic structure techniques to develop an understanding of their intrinsically dynamic behaviour. We study the rich kinetics of the rotation of the organic cation by applying careful analysis to ab-initio molecular dynamics simulations [1]. Informed by observations of the dynamics, a on-lattice model model is developed to access far longer length and timescales of the dynamic system. Parameterisation of the Hamiltonian is from electronic structure calculations. This model shows columnar anti-ferroelectric and ferroelectric ground states, as a function of strain and lattice distortion energetics. The transition from short range to long range order as a function of temperature is analysed by defining & measuring correlation functions. The electrostatic potential is reconstructed from dipole orientation. A model for polaronic transport and recombination in the material is developed, where the low electron recombination rates in these materials is related to the columnar structure of the electrostatic potential leading to electron and hole segregation.

1. J.M. Frost, K. Butler, A. Walsh, APL Materials 2 (8), 081506 (2014).

CPP 60.8 Thu 12:00 C 130

**Quantum-Chemical Calculations of Hybrid Perovskites** — •Wichard J. D. Beenken, Ksenia Korschunova, Mezhoura Oussadou, Lars Winterfeld, and Erich Runge — Institut für Physik und Institut für Mikro- und Nanotechnologie, Technische Universität Ilmenau, Germany

Hybrid perovskites possess a multitude of structural phases depending on temperature and the organic cations. Thus a deeper understanding of the various crystal structures and their influence on the electronic bandstructure is necessary to control the quality of these materials for solar cells. Though there exist already several structure analyses of perovskites by X-ray diffraction, the severe problem remains that the contrast of organic light atoms (C, N, H) and inorganic heavy atoms (Pb, I) is several magnitudes. This makes it difficult to determine the exact positions of the organic cations within the perovskite lattice spanned by a network of octahedral Lead-Iodid anions. Consequently, most of the published structures for hybrid perovskites do only provide guesses for the organic part, in particular for the H-atoms. Their positions, however, may be important for understanding the electronic band structure, which is also difficult to be determined experimentally, e.g. by angle resolved UPS, for the polycrystallinity of the samples. Therefore, we have done DFT calculations using the quantum-chemical package VASP 5.3for crystal structure optimization and band structure determination of low-temperature and metastable phases of several organic-inorganic hybrid perovskites.

CPP 60.9 Thu 12:15 C 130

**Radiative efficiency of perovskite solar cells** — •Kristofer Tvingstedt[1], Olga Malinkiewicz[2], Andreas Baumann[3], Carsten Deibel[1], Henry J. Snaith[4], Vladimir Dyakonov[1,3], and Henk J. Bolink[2] — [1]Experimental Physics VI, Julius-Maximillian University of Würzburg, 97074 Würzburg, Germany — [2]Instituto de Ciencia Molecular, Universidad de Valencia, 46980 Paterna, Valencia, Spain — [3]Bavarian Center for Applied Energy Research, 97074 Würzburg, Germany — [4]University of Oxford, Clarendon Laboratory, Parks Road Oxford, OX1 3PU, United Kingdom

Perovskite PVs have reached significant power conversion efficiency in a very short time period. Apart from providing a rather high photocurrent, they also retain a comparatively high open circuit voltage. We here address the upper limit to open circuit voltage and power conversion efficiency for the novel type of photovoltaic cells based on methylammonium lead iodide perovskites. By accurate determination of the present solar cells radiative efficiency, that is their ability to emit light, we conclude how far these solar cells are from their own thermodynamic limit. We explain the reason for the high voltage and put it in relation to those of earlier generation photovoltaic technologies. We further highlight that, as the perovskite steady state photoluminescence is rather strong at open circuit conditions, and substantially quenched only at short circuit, they perform just as good solar cells should do, and in this respect also rather different from most OPVs or DSSC cells studied so far.

CPP 60.10 Thu 12:30 C 130

**Recombination behaviour of hybrid perovskite thin films studied by low temperature photoluminescence** — Sergej Levcenco, Amrita Mandal Bera, Dan Wargulski, Ibrahim Simsek, and •Thomas Unold — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner Platz 1, 14109 Berlin

Hybrid organometal perovskites recently have been successfully implemented as absorber layers in high efficiency thin film solar cells. In particular the CH3NH3PbI3 based materials show long minority carrier recombination lifetimes, implying a minor role of non-radiative recombination even at room temperature. In order to better understand the radiative recombination properties we have studied hybrid perovskite layers on glass, which where pepared by immersion of polycrystalline PbI2- thin films into methylammoniumiodide dissolved in isopropanol. The perovskite layers show high luminescence efficiencies at room temperature with a broad peak centered at around 1.6eV. At low temperature, several additional transitions are observed, which shift with temperature and show significant thermal quenching. Changes in the radiative emission caused by degradation of the layers under ambient conditions will also be reported.

CPP 60.11 Thu 12:45 C 130

**Transient electrical studies probing charge carrier recombination in methylammonium lead iodide perovskite solar cells** — •Andreas Baumann[1], Stefan Väth[2], Kristofer Tvinstedt[2], Michael C. Heiber[2], Cristina Momblona[3], Henk J. Bolink[3], and Vladimir Dyakonov[1,2] — [1]Bayerisches Zentrum für Angewandte Energieforschung, Am Galgenberg 87, D-97074 Würzburg — [2]Experimentelle Physik 6, Julius-Maximilians-Universität Würzburg, Am Hubland, D-97074 Würzburg — [3]Universidad de Valencia, Paterna, Spain

Organo-metal halide perovskites like methylammonium lead iodide show extraordinary photovotlaic performance with power conversion efficienies exceeding 20%. However, a fundamental understanding of the physical processes in perovskite solar cells is still lacking but is essential for further development in this quickly emerging research field. Here, we present our recent studies on the charge carrier recombination in methylammonium lead iodide perovskite solar cells in a planar configuration without porous transport layers by means of open circuit voltage decay measurements. The results are compared with the recombination behavior in reference state-of-the-art polymer-fullerene bulk heterojunction solar cells.[1] We observed two very different time domains in the transients of the perovskite solar cells in contrast to the organic reference solar cells. We will discuss potential origins of these unique behavior and compare the results for various device configurations.[1] A. Baumann et al., APL Mater. 2, 081501 (2014)

# CPP 61: Focus: Disordered Systems, Glasses under Shear I (joint session CPP, DY)

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

**Invited Talk** CPP 61.1 Thu 9:30 C 243

**Flow instabilities in soft glassy materials** — •Suzanne Fielding — Department of Physics, Durham University, UK

Many soft materials, including dense emulsions, microgel suspensions, star polymers, onion surfactants, and textured morphologies of liquid crystals, share underlying glassy features of structural disorder and metastability. These give rise to several notable features in the low frequency rheology of these materials: for example, the existence of a yield stress below which the material behaves like a solid, and above which it flows like a liquid. Experiments have also revealed that these materials often display a phenomenon known as shear banding, in which the flow profile across the shear cell exhibits macroscopic bands of different viscosity. Two distinct classes of yield stress fluid have been identified: those in which the shear bands apparently persist permanently (for as long as the flow is applied), and those in which banding arises only transiently during a process in which a steady flowing state is established out of an initial rest state (eg in shear startup or step stress). After surveying this motivating experimental data, we describe recent progress in addressing it theoretically, using the soft glassy rheology model and a simple fluidity model. Time permitting we shall also discuss failure modes of these "soft glassy materials" in free-surface extensional flows.

CPP 61.2 Thu 10:00 C 243

**Shear cessation in a Brownian-dynamics simulation for 2D hard disks** — •Sebastian Fritschi and Matthias Fuchs — Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

We present results from a Brownian-dynamics computer simulation for the nonequilibrium transient dynamics in a colloidal glass former after the cessation of shear flow. In the glass, persistent residual stresses are found that depend on the flow history. The partial decay of stresses from the steady state to this residual stress is governed by the previous shear rate. Using a glassy hard-disk system, we also link this macroscale dynamics to microscopic particle motion, monitoring the transient mean-squared displacement measured during the relaxation from the steady state. A flow-induced second plateau is found in the mean-squared displacement at long times.

CPP 61.3 Thu 10:15 C 243

**Microrheology of a Two-Dimensional Driven Granular System** — •Peidong Yu, Boris Eberhardt, Sebastian Pitikaris, and Matthias Sperl — Institut für Materialphysik im Weltraum, Deutches Zentrum für Luft- und Rahmfahrt, Köln, Deutschland

We study the motion of a tracer particle pulled inside a two-dimensional granular model system, where particle movements can be controlled and precisely tracked. We put such a system on a shaking table and apply vertical agitation as thermalization. We show how well the particles are themalized in the horizontal direction. We then drag a tracer particle through such a system with constant force or constant velocity. Effective viscosities with different parameters are measured. Different scenarios of shear thinning and shear thickening are observed. The underlying physics is discussed and compared with simulations and theories.

CPP 61.4 Thu 10:30 C 243

**Potential energy landscape analysis of sheared glass-forming systems** — •Markus Blank-Burian and Andreas Heuer — Institut für Physikalische Chemie, WWU Münster, Deutschland

We performed molecular dynamics simulations of small binary Lennard-Jones mixtures ($65 \leq N \leq 1040$) under constant shear rates and at a very low temperature ($T = 0.01$). The shearing is achieved by applying Lees-Edwards periodic boundary conditions to the system.

In previous work on unsheared systems it was shown, that most of the physical properties of macroscopic systems are already encoded in these small systems. The dynamics of these small systems can be described by a continous time random walk (CTRW) between minima of the potential energy landscape (PEL). Our focus now lies on comparing these results with the constantly sheared system.

For the analysis of the sheared system, we perform energy minimization using the strain as an additional variable. We then use this information to identify inherent structures (IS) from the trajectories. These IS turn out to have zero strain. Thus, they are comparable to the unsheared system. From the resulting statistical data we hope to gain a microscopic understanding of macrorheological phenomena like the initial stress overshoot as well as the shear thinning in the plastic flow regime.

**Invited Talk** CPP 61.5 Thu 10:45 C 243

**Dense granular flow** — •Annette Zippelius — Institut für Theo. Physik, Univ. Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen

In the first part of the talk I will discuss a jamming scenario of frictional particles, which can be interpreted as a nonequilibrium first order phase transition (1). Results of numerical simulations will be presented and analyzed in the framework of a simple model which can account for both, the continuous frictionless case and the discontinuous frictional case. The most important features of the frictional phase diagram are reentrant behaviour and a critical jamming point at finite stress.

The second topic to be discussed are dynamical heterogeneities and scaling in a driven granular fluid as structural arrest is approached (2). Large scale simulations of 2d bidisperse granular fluids allow us to determine spatial correlations of slow particles via the four-point structure factor. As the fluid approaches structural arrest, scaling is shown to hold. Both the dynamic susceptibility as well as the dynamic correlation, evaluated at the alpha-relaxation time,can be fitted to a power law divergence at a critical packing fraction. The measured susceptibility widely exceeds the largest one previously observed for hard sphere 3d fluids. The clusters of slow particles are neither compact nor stringlike but fractal. The cluster size distrbution is shown to fall off algebraically as structural arrest is approached.

(1) M. Grob, C. Heussinger and A. Zippelius, Phys. Rev E 89, 050201 (R) (2014); (2) K. Avila, H. C. Castill, A. Fiege, K. Vollmayr-Lee and A.Zippelius, Phys. Rev. Lett. 113, 025701 (2014)

**15 min. break**

CPP 61.6 Thu 11:30 C 243

**Transient Rheology of Colloidal Suspensions - Shear Reversal** — •Miriam Siebenbürger[1], Fabian Frahsa[2], and Matthias Fuchs[2] — [1]Helmholtz Zentrum Berlin, Germany — [2]Universität Konstanz, Germany

At low deformations, colloidal glasses exhibit first a linear deformation, followed by a stress overshoot and the sheared steady state [1]. In this transition range from solid to fluid the reversal of the shear deformation can spend insights in the dynamics of the underlying structural transformations. Experimental investigations are performed by model suspension of thermo-sensitive colloids, consisting of a poly(styrene) core and a poly(N-isopropylacrylamide) shell. By a set of shear reversal experiments the aging effect often observed in experimental systems can be discussed separately from the structural transformations due to the shear. The height and the position of the minimum of the undershoots in the reversed shear flow is correlated with the deformation at the start of the shear reversal. All results for different shear rates and waiting times will be compared to the Mode Coupling Theory (MCT) and simulations, which show good agreement compared to the experimental results [2].

[1] C. P. Amann, F. Weysser, M. Fuchs, M. Siebenbürger, M. Krüger and M. Ballauff, J. Rheol. 57,149 (2012).

[2] F. Frahsa, A. Bhattacharjee, J. Horbach, M. Fuchs and T. Voigtmann, J. Chem. Phys. 138, 12A513 (2013).

CPP 61.7 Thu 11:45 C 243

**Lattice Boltzmann Simulations of Glass Forming Liquids** — •Simon Papenkort[1] and Thomas Voigtmann[1,2] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln — [2]Heinrich-Heine-Universität Düsseldorf

The rheology of complex fluids undergoing a glass transition, such as colloidal suspensions or granular media, is highly nonlinear. The interplay between slow structural dynamics on the microscopic scale and a mesoscopic flow field gives rise to non-Newtonian flow effects. Prominent examples are shear thinning, dynamic yield and residual stresses. In a confined flow geometry, the shear rates, and thereby the fluid properties, can vary considerably in space and time. Even long after the flow has stopped, the material properties are profoundly affected by residual stresses.

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. The Lattice Boltzmann method is a modern simulation scheme to solve the Navier-Stokes equations even for complex flow geometries. We introduce a new, modified LB model [1] which is able to include memory-integral effects in fluid-mechanics simulations and provides a link between both regimes.

We find the viscoelastic transient dynamics and the appearance of residual stresses after stopping the flow to depend sensitively on the chosen flow geometry.

[1] J. Chem. Phys. 140, 164507 (2014)

CPP 61.8 Thu 12:00 C 243

**Shear bands at the Jamming Transition: The role of Weak Attractive Interactions** — •Ehsan Irani[1], Pinaki Chaudhuri[2], and Claus Heussinger[1] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany — [2]Institute of Mathematical Sciences, Tamil Nadu, India

We study the rheology of a particulate sytem close to Jamming in the presence of weakly attractive interactions. Lees-Edwards boundary conditions are used to simulate a shear-controlled flow. In addition to Bagnold scaling at large shear rates, the attraction results in a finite yield stress in the limit of small shear rates. In the yield regime a fragile solid is formed and the rheology can be explained by a scaling argument that exploits the vicinity to the isostatic state. In the transition region the shear stress develops a minimum, which (in large enough systems) leads to the formation of persistent shear bands. These features are rationalized by a scenario that involves the competition between attraction-induced structure formation and its break-down because of shearing. Properties of shear bands are studied in order to reveal the physical mechanisms that underly the non-monotonic flow curve and the flow heterogenities in the transition region. This work may help to elucidate the origin of shear bands in different materials with finite and short-ranged attractive forces.

CPP 61.9 Thu 12:15 C 243

**Influence of drops on particles under shear** — •Laurent Gilson, Jennifer Wenzl, and Günter Auernhammer — Max Planck Institute for Polymer Research, Physics at Interfaces, Mainz

We will present shear zone formation in granulates with and without the influence of liquid droplets. 3D Laser Scanning Confocal Microscopy (LSCM) was used to image polydisperse spherical silica particles (7$\mu$m) during quasi-steady strain controlled shear experiments.A shear cell was formed using a fixed bottom plate and a nanoindenter tip [1]. This arrangement creates a strain-controlled shear cell without lateral walls. Samples consisted of polydisperse spherical silica particles suspended in an index matching liquid. Immiscible droplets were used as a second phase. Position and form of the droplets, as well as position and size of the particles were recorded simultaneously using a dual channel LSCM [1,2,3]. Multiple images were taken during shear. A complete record of individual particle and droplet movement during shear was extracted.

We will focus our presentation on the differences between particles attached to droplets and particles in bulk. We will discuss differences and common features, as well as compare the results to features commonly found in sheared granular matter.

[1] Wenzl, J., Seto, R., Roth, M., Butt, H.-J., Auernhammer, G., Granul. Matter, 15, 391-400 (2012). [2] Crocker, J.C., Grier, D.G, J. Colloid Interface Sci. 179(1), 298-310 (1996). [3] Roth, M., Schilde, C., Lellig, P., Kwade, A., Auernhammer, G., Eur. Phys. J. E, 35(11), 124 (2012)

CPP 61.10 Thu 12:30 C 243

**Shear bands in a model glass former** — •Gaurav Prakash Shrivastav[1], Pinaki Chaudhuri[2], and Jürgen Horbach[1] — [1]Institut für Theoretische Physik II - Soft Matter, Heinrich-Heine-Universität Düsseldorf, Germany — [2]The Institute of Mathematical Sciences, Chennai, India

We study the mechanical response of a binary Lennard-Jones mixture by shearing it below the glass transition temperature with a constant strain rate. The onset of flow is associated with an inhomogeneous flow pattern [1,2]. Highly mobile regions form a long-lived shear-band-like structure. Although the flow curve is monotonic and stress-strain response does not show any signature of a shear band, this heterogeneity is captured very well in the mean square displacement of particles. The width of the shear band grows diffusively with time. We find that shear bands are more pronounced in the cuboid boxes than in the cubic boxes. This can be explained by the quadrupolar structure of the local strain fields. To investigate the origin of shear bands we identify the local events that lead to their formation. We observe that these initial active spots are localized to one or two particles.

[1] P. Chaudhuri, J. Horbach, Phys. Rev. E **88**, 040301(R) (2013).

[2] P. Chaudhuri, J. Horbach, Phys. Rev. E **90**, 040301(R) (2014).

CPP 61.11 Thu 12:45 C 243

**Creep deformation of glasses under shear stress, results from a schematic mode-coupling model** — •Fabian Frahsa and Matthias Fuchs — Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

The viscoelasticity of dense colloidal dispersions causes creep deformation under constant stress. Creep provides insight in the slow structural dynamics and dissipative processes of glasses.

We present predictions for the stress-driven rheology of glass from a schematic model of the mode-coupling theory (MCT) and compare them with experiments of core-shell micro gels. The schematic model is motivated by the microscopic ITT-MCT approach to the stress response of flow-driven systems and covers incompressible and homogeneous flows neglecting hydrodynamic interactions.

## CPP 62: Complex Fluids and Soft Matter - Part II (joint session DY, CPP, BP)

Time: Thursday 9:30–11:45 Location: BH-N 334

**Invited Talk** CPP 62.1 Thu 9:30 BH-N 334

**Ultrasoft particles under out-of-equilibrium conditions** — •Gerhard Kahl — Institut für Theoretische Physik, TU Wien, Vienna, Austria

On a coarse-grained level, colloids often interact via so-called ultrasoft potentials, which assume at short interparticle distances values in the order of a few $k_{\mathrm{B}}T$; thus, these particles are able to overlap at the cost of a relatively small energy penalty. Under equilibrium conditions such ultrasoft particles are able to form aggregates (clusters) of overlapping particles which can then either form a disordered or an ordered cluster phase. In the latter case, these aggregates populate the positions of a regular fcc or bcc lattice. Cluster crystals display rather unconventional properties, such as a density-independent lattice constant [1]. Also under out-of-equilibrium conditions, ultrasoft systems show unexpected features. Exposing a cluster crystal to shear leads – with increasing shear rate $\dot{\gamma}$ – to the following novel response-scenario: for small $\dot{\gamma}$-values the crystal melts; then gradually strings parallel to the flow direction form which are arranged in a hexagonal grid in the gradient-vorticity plane. Upon further increasing $\dot{\gamma}$ this lattice eventually melts [2]. Exposing a cluster crystal to Poiseuille flow the emergence of a quantized flow pattern is observed where the height and the width of the fluid stream display well-defined plateaus, indicating a successive fluidization of crystal layers adjacent to the channel walls [3].

[1] B.M. Mladek *et al.*, Phys. Rev. Lett. **96**, 045701 (2006).

[2] A. Nikoubashman *et al.*, Phys. Rev. Lett. **107**, 068302 (2011).

[3] A. Nikoubashman *et al.*, Soft Matter **8**, 4121 (2012).

CPP 62.2 Thu 10:00 BH-N 334

**Dynamics of density excitations in shear-driven, confined binary mixtures** — •Sascha Gerloff, Tarlan A. Vezirov, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

Understanding friction on the microscopic scale is of great interest both from a fundamental and an applicational point of view. An important topic in this context is the appearance of density heterogeneities [1].

Here we perform overdamped Brownian dynamics simulations of a thin film of charged colloidal particles with two different sizes in planar shear flow. The particles interact via a combined Yukawa- and softsphere-potential. The parameters are set to suit experimental data for ludox silica particles, which where previously studied. The one-component system is known to form shear-induced multi-layer configurations in confinement and to show different intra-layer structures which depend on the applied shear rate. [2]

The corresponding two-component system under shear displays density excitations, provided that mixing of the two species is prohibited. We investigate the distribution and motion of these density excitations using voronoi tessellation. The density excitations are then identified as clusters of high local density in the spirit of the Hoshen-Kopelman algorithm.

[1] T. Bohlein, J. Mikhael and C. Bechinger, Nat. Mater. 11, 126-130 (2012).

[2] T. A. Vezirov and S. H. L. Klapp, Phys. Rev. 88, 052307 (2013).

CPP 62.3 Thu 10:15 BH-N 334

**Analytical solutions for immiscible two-phase-flow in porous media** — •Christoph Wolber and Rudolf Hilfer — Institut für Computerphysik, Universität Stuttgart, Allmandring 3, 70569 Stuttgart

A macroscopic theory for two-phase-flow in porous media that distinguishes between percolating (free-flowing) and non-percolating (trapped, disconnected) fluid parts has been studied. The theory naturally predicts hysteresis and spatiotemporal variations of residual and irreducible saturations. The computational advantage of the generalization over the traditional theory is the strict locality in time of all processes including hysteretic processes with simultaneous drainage and imbibition. Initial and boundary value problems on semi-infinite domains with constant total flux (generalized Buckley Leverett problems) have been solved semi-analytically with and without flow reversal. Complex combinations of shock fronts and rarefaction waves have been observed as the result.

CPP 62.4 Thu 10:30 BH-N 334

**Saturation overshoot and hysteresis for twophase flow in porous media** — •Rouven Steinle and Rudolf Hilfer — Institute for Computational Physics, University of Stuttgart, Germany

Observations of non-monotone saturation profiles (saturation overshoot) during twophase infiltration processes have recently attracted much attention because such profiles are mathematically excluded within the Richards approximation to the traditional Darcy theory. Here it is shown that a traditional Darcy theory combined with a simple hysteresis model yields non-monotone saturation profiles in the Buckley-Leverett limit. Analytical arguments and numerical simulations are reported. They agree quantitatively in predicting saturation overshoot. A simple jump-type hysteresis in the relative permeabilities suffices to yield a saturation overshoot, while hysteresis in the capillary pressure is not needed [1]. Extensive numerical simulations of the mathematical model reveal a strong dependence of the overshoot phenomenon on the initial and boundary conditions.

[1] Hilfer, R. and Steinle, R., *Saturation overshoot and hysteresis for twophase flow in porous media*, Eur.Phys.J.ST, vol. 223, pp. 2323 (2014)

CPP 62.5 Thu 10:45 BH-N 334

**Free energy cost of forming a solid-liquid interface** — •Ronald Benjamin[1] and Jürgen Horbach[2] — [1]Institut für Theoretische Physik II - Soft Matter, Heinrich-Heine-Universität, 40225 Düsseldorf — [2]Institut für Theoretische Physik II - Soft Matter, Heinrich-Heine-Universität, 40225 Düsseldorf

Knowledge of the solid-liquid interfacial free energy is crucial to an understanding of nucleation, crystallization, and wetting phenomena. In this talk, we present a novel simulation technique to compute this quantity directly for an interface between a crystal and its melt [1]. Our approach solves an important problem arising out of hysteresis effects which led to uncontrolled errors in previous studies. We apply our method to different interaction potentials [1, 2] and do a careful finite-size scaling analysis in each case to obtain reliable estimates of the solid-liquid interfacial free energies.

Reference:-

1.) Crystal-liquid interfacial free energy via thermodynamic integration.-R. Benjamin and J. Horbach, J. Chem. Phys. 141, 044715 (2014).

2.) Crystal-liquid interfacial free energy of hard spheres via a novel thermodynamic integration scheme.- R. Benjamin and J. Horbach, arXiv 1410.8798 (2014).

CPP 62.6 Thu 11:00 BH-N 334

**Transient microrheology of viscoelastic fluids** — •Juan Ruben Gomez Solano[1,2] and Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universitaet Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Max-Planck-Institute for Intelligent Systems, Heisenbergstrasse 3, 70569 Stuttgart, Germany

Viscoelasticity is ubiquitous in soft matter ranging from biological fluids to new synthetised materials, whose mechanical response deviate from Newtonian behavior under applied stress or strain. Microrheology has proved successfully in recent years as an alternative to bulk rheology in investigating linear and steady-state flow properties of microlitre samples of such materials. More complex transient behavior, e.g. creep and strain recovery after flow startup and cessation, is far less well understood within the context of microrheology. In this work we experimentally study the transient motion of a colloidal particle actively dragged by an optical trap through different viscoelastic fluids (wormlike micelles, polymer solutions, and entangled lambda-phage DNA). We observe that, after sudden removal of the moving trap, the particle recoils due to the relaxation of the deformed fluid microstructure until its complete strain recovery. We find that the relaxational dynamics of the particle proceeds via a double exponential decay, whose relaxation times remain independent of the initial particle velocity whereas their amplitudes strongly depend on it. We show that this transient information, which has no counterpart for colloids moving in Newtonian fluids, can be exploited to determine linear and non-linear flow properties of the embedding fluid.

CPP 62.7 Thu 11:15 BH-N 334

**Flow properties of anisotropic fluids** — •Sebastian Heidenreich[1], Sabine H. L. Klapp[2], and Markus Bär[1] — [1]Physikalisch Technische Bundesanstalt, Berlin, Germany — [2]Technische Universität Berlin, Germany

From liquid crystal polymers to suspensions of bacteria anisotropic fluids are ubiquitous in nature and technology. The flow exhibits intriguing phenomena like flow alignment, shear banding, tumbling, shear thickening/thinning, large-scale correlation and mesoscale turbulence. The emergence of such fascinating aspects is often related to the anisotropy and to the out-of equilibrium character of the considered system. In the first part of our presentation we review selected flow phenomena of passive fluids with anisotropy. We discuss the role of the order parameter like the alignment tensor for the description of the flow properties. In particular, we introduce the relaxation equation for the alignment tensor coupled to the hydrodynamic flow and discuss the orientational dynamics in the shear flow. In the second part of the talk we focus on active fluids like dense bacterial suspensions and we introduce the governing hydrodynamic equations for self-sustained individuals that are swimming in a Newtonian fluid. We discuss the relationship to the passive counterpart and finally present recent work on mesoscale bacterial turbulence.

**15 min. break**

# CPP 63: Cytoskeletal filaments (Joint session BP, CPP)

Time: Thursday 9:30–13:00 Location: H 1028

**Invited Talk** CPP 63.1 Thu 9:30 H 1028

**Microtubules adapt to mechanical stress through spontaneous intra-lattice repair** — Laura Schaedel[1], Karin John[1], Jeremie Gaillard[1], Maxence Nachury[2], Laurent Blanchoin[1], and •Manuel Thery[1,3] — [1]UMR5168, CEA/CNRS/INRA/Université Grenoble-Alpes, Grenoble, France — [2]Stanford University School of Medicine, CA 94305, USA. — [3]Hôpital Saint Louis, UMRS1160, INSERM/AP-HP/Université Paris Diderot, Paris, France

Microtubule arrays define the shape of axons, cilia and flagella, and provide tracks for intracellular transport. Although microtubules assembled in vitro are stiffer than other cytoskeletal polymers by several orders of magnitude, intracellular forces lead to the formation of highly bent microtubules. It is currently not known how microtubules tolerate the vast forces exerted on them. It is likely that physical constraints affect microtubule structure and stiffness. Using a newly developed microfluidic device, we find that microtubule stiffness decreases incrementally with each cycle of bending and release. Similar to other cases of material fatigue, rather than a homogenous distribution of stress, the concentration of mechanical stresses turns pre-existing defects in the microtubule lattice into larger damages. Strikingly, damaged microtubules are able to recover their initial stiffness by spontaneously incorporating tubulin into their lattice. These findings demonstrate that microtubules are ductile materials with self-healing properties. Microtubule dynamics is thus not exclusive to the ends and intra-lattice incorporation of tubulin enables spontaneous adaptation to mechanical stresses.

CPP 63.2 Thu 10:00 H 1028

**Molecular wear of microtubules propelled by surface-adhered kinesins** — Emmanuel LP Dumont[1], Catherine Do[2], and •Henry Hess[1] — [1]Department of Biomedical Engineering, Columbia University, New York, New York 10027, USA — [2]Institute for Cancer Genetics, Columbia University Medical Center, New York, New York 10032, USA

Wear, the progressive loss of material from a body caused by contact and relative movement, is a major concern not only in engineering but also in biology. Advances in nanotechnology both enable the study of the origins of wear processes at the atomic and molecular scale and demand the prediction and control of wear in nanoscale systems. Here we discuss wear that occurs in an in vitro system consisting of microtubules gliding across a surface coated with kinesin-1 motor proteins, and that energetic considerations suggest a molecule-by-molecule removal of tubulin proteins. The rates of removal show a complex dependence on sliding velocity and kinesin density, which - in contrast to the friction behavior between microtubules and kinesin - cannot be explained by simple chemical reaction kinetics.

CPP 63.3 Thu 10:15 H 1028

**Diffusible crosslinkers generate directed forces in microtubule networks** — Zdenek Lansky[1,2,5], •Marcus Braun[1,2,5], Annemarie Lüdecke[1,2], Michael Schlierf[1], Pieter Rein ten Wode[3], Marcel Janson[4], and Stefan Diez[1,2] — [1]B CUBE, TU Dresden, Germany — [2]MPI-DBG, Dresden, Germany — [3]AMOLF, Amsterdam, The Netherlands — [4]Laboratory of Cell Biology, Wageningen University, The Netherlands — [5]equal contribution

Remodeling of cytoskeletal filament networks is essential to cell division and morphogenesis. The mechanical forces driving the restructuring are attributed to the action of molecular motors and filament dynamics, which both consume chemical energy. By contrast, non-enzymatic filament crosslinkers are regarded as mere friction-generating entities. Here, we experimentally demonstrate that non-enzymatic, diffusible microtubule crosslinkers of the Ase1/PRC1/Map65 family generate directed microtubule sliding when confined between partially-overlapping microtubules. The Ase1-generated forces, directly measured by optical tweezers to be in the piconewton-range, were sufficient to antagonize motor-protein driven microtubule sliding. Force generation can be quantitatively explained by the entropic expansion of confined Ase1 molecules diffusing within the microtubule overlaps. The thermal motion of confined crosslinkers is thus harnessed to generate mechanical work analogous to compressed gas propelling a piston in a cylinder. As confinement of diffusible crosslinkers is ubiquitous in cells, the associated entropic forces are likely to be of importance for cellular mechanics beyond cytoskeletal networks.

CPP 63.4 Thu 10:30 H 1028

**The Dynamics of cross-linked Microtubules in Neurons** — •Maximilian Jakobs — University of Cambridge — Universität zu Köln

Microtubule bundles play a central role in the initiation and growth of cellular processes such as neuronal axons and dendrites. However, a quantitative understanding of the involved mechanisms is still lacking. Here, we developed computer simulations that mimic the 1D dynamics of microtubule bundles, cross-linked by ensembles of molecular motors, to investigate the mechanics of growth. We demonstrated that unipolar motors (such as cytoplasmic dynein and most kinesins) are much more effective in initiating axon growth than bipolar motors (such as kinesin 5). The latter, however, are in turn more efficient in filament sorting. We furthermore investigated axon growth dynamics as a function of the restoring forces acting on MT bundles. Our calculations demonstrated that the maximum force such bundles may exert increases monotonically with the elastic rigidity of the opposing membrane, and that it is insensitive to the polarity of filaments in the bundle. Finally, we found that the motor density must exceed a percolation threshold, which depends on the number of filaments in the bundle, before any force can be exerted. Future experiments and considerations might reveal an important contribution of microtubule-generated forces to neuronal symmetry breaking.

CPP 63.5 Thu 10:45 H 1028

**Cross-linking proteins facilitate formation of microtubule bundles** — •Marcel Prelogovic[1], Lora Winters[2], Iva Tolić[2], and Nenad Pavin[1] — [1]Faculty of science , University of Zagreb, Croatia — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

During mitosis, microtubules (MTs) form a spindle which is responsible for proper segregation of chromosomes. In the fission yeast Schizosaccharomyces Pombe, the spindle is a bundle of MTs emanating from two spindle pole bodies and held together by cross-linking proteins. Our goal is to understand the dynamic properties of MTs interacting with cross-linking proteins and the role of cross-linking proteins in the formation of MT bundles. We introduce a theoretical model of MT bundling which describes angular movement of MTs around the spindle pole body driven by thermal forces and forces exerted by cross-linking proteins, described as elastic springs. If the number of cross-linking proteins connecting the MTs is above a critical number, attractive forces exerted by cross-linking proteins dominate over thermal forces at very small angles between MTs, causing MT-s to bundle. We identify stable bundles as the cases where MTs are more likely to be bundled than not. Theory yields bundling probability as a function of length and cross-linking protein concentration and predicts parameters for which stable bundles form. In conclusion, these results provide an explanation for how the angular brownian motion and cross-linking proteins affect the formation of stable MT bundles.

CPP 63.6 Thu 11:00 H 1028

**Quantifying protein diffusion and capture on filaments** — •Emanuel Reithmann, Louis Reese, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität, München

The functional relevance of regulating proteins is often restricted to specific binding sites such as the ends of microtubules or actin-filaments. A localization of proteins on these functional sites is of great importance. In this respect, recent experimental studies suggested that several key players involved in regulation of microtubules and actin-filaments utilize a one-dimensional diffusive motion on the respective filament to target the functional end. We present a quantitative theory for a diffusion and capture process, where proteins diffuse on a filament and stop diffusion when reaching the filament's end. It is found that end-association after one-dimensional diffusion is highly efficient as compared to direct binding from solution/cytoplasm. As a consequence, diffusion and capture substantially enhances the reaction velocity of enzymatic reactions, where proteins and filament ends are to each other as enzyme and substrate. We show that the reaction velocity ensuing from diffusion and capture can effectively be computed within a Michaelis-Menten framework. We predict that diffusion and capture would significantly beat the (three-dimensional) Smoluchowski diffusion limit for the rate of direct protein association to filament ends for practically all proteins that are known to diffuse on microtubules and actin-filaments.

**15 min break**

**Invited Talk** CPP 63.7 Thu 11:30 H 1028

**Cellular chirality arising from the self-organization of the actin cytoskeleton** — •Alexander Bershadsky — Department of Molecular Cell Biology, Weizmann Institute of Science, Rehovot 76100, Israel — Mechanobiology Institute, National University of Singapore, Singapore 117411, Singapore

Cellular mechanisms underlying the development of left-right asymmetry in tissues and embryos remain obscure. Here, the development of a chiral pattern of actomyosin was revealed by studying actin cytoskeleton self-organization in cells with isotropic circular shape. A radially symmetrical system of actin bundles consisting of $\alpha$-actinin-enriched radial fibers (RFs) and myosin-IIA-enriched transverse fibers (TFs) evolved spontaneously into the chiral system as a result of the unidirectional tilting of all RFs, which was accompanied by a tangential shift in the retrograde movement of TFs. We showed that myosin IIA-dependent contractile stresses within TFs drive their movement along RFs, which grow centripetally in a formin-dependent fashion. The handedness of the chiral pattern was shown to be regulated by $\alpha$-actinin-1. Computational modeling demonstrated that the dynamics of radial-transverse fiber system can explain the pattern transition from radial to chiral. Thus, actin cytoskeleton self-organization provides built-in machinery that potentially allows cells to develop left-right asymmetry.

CPP 63.8 Thu 12:00 H 1028

**Spontaneous polarization in an interfacial growth model for actin filament networks with a rigorous mechanochemical coupling** — •Karin John[1], Denis Caillerie[2], Thomas Stoeter[1,3], and Chaouqi Misbah[1] — [1]Université Grenoble Alpes/ CNRS, LIPHY, F-38000 Grenoble, France — [2]Université Grenoble Alpes/CNRS, 3SR, F-38000 Grenoble, France — [3]Otto-von-Guericke Universität Magdeburg

Many processes in eukaryotic cells, including cell motility, rely on the growth of branched actin networks from surfaces. Despite its central role the mechanochemical coupling mechanisms that guide the growth process are poorly understood, and a general continuum description combining growth and mechanics is lacking. We develop a theory that bridges the gap between mesoscale and continuum limit and propose a general framework providing the evolution law of actin networks growing under stress. This formulation opens an area for the systematic study of actin dynamics in arbitrary geometries. Our framework predicts a morphological instability of actin growth on a rigid sphere, leading to a spontaneous polarization of the network with a mode selection corresponding to a comet, as reported experimentally. We show that the mechanics of the contact between the network and the surface plays a crucial role, in that it determines directly the existence of the instability. We extract scaling laws relating growth dynamics and network properties offering basic perspectives for new experiments on growing actin networks.

CPP 63.9 Thu 12:15 H 1028

**Contractile actin bundles without molecular motors** — •Jörg Schnauss[1], Tom Golde[1], Carsten Schuldt[1], Sebastian Schmidt[1], Martin Glaser[1], Dan Strehle[1], Josef Käs[1], and Claus Heussinger[2] — [1]Institute for Experimental Physics I, University of Leipzig , Linnéstraße 5, 04103 Leipzig , Germany — [2]Institute for Theoretical Physics, Georg-August University of Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen, Germany

Since the 1940, interactions of actin and its molecular motor myosin are known as the fundamental process for biological force generation. These interactions convert chemical energy into mechanical work by ATP hydrolysis. The dogma of molecular motors being the basis of all contractile forces has never been disproven. In this study we show an alternative force generation mechanism in the absence of molecular motors. The system is not driven by ATP hydrolysis and solely relies on minimization of free energy based on filament-filament interactions induced by a crowded environment. Dynamics of these contractions behave differently to a single filament pair shown in theoretical and experimental studies. We are able to show that the behavior of contractile actin bundles can be well described as an emergent phenomenon of multiple filament pairs. This crowding regime is well below the macromolecular content of cells and crowding effects have to be considered in cellular systems. We measured contraction velocities ranging from 0.10 to 0.65 $\mu$m/s and evaluated a force regime of 0.5 to 3.0 pN. Dynamics and forces of this non-dissipative process correspond to an active behavior of single myosin motors.

CPP 63.10 Thu 12:30 H 1028

**Organisation dynamics of stress fibers in adult stem cells** — •Carina Wollnik[1], Benjamin Eltzner[2], Stephan Huckemann[2], and Florian Rehfeldt[1] — [1]Third Institute of Physics - Biophysics, Georg-August-University, Göttingen, Germany — [2]Institute for Mathematical Stochastics, Georg-August-University, Göttingen, Germany

Adult human mesenchymal stem cells (hMSCs) differentiate into various cell types. Here substrate stiffness is sufficient to guide hMSCs towards different lineages without additional biochemical stimuli [1]. Stress fibres (SFs)composed of actin filaments, cross-linkers and myosin motor-proteins generate and transmit tension throughout the cell. Myosin inhibition stops the differentiation [1], implying importance of SF tension for this process. Characteristic SF patterns can be detected within 24 hours and used as an early morphological marker [2].

We use 24h long-term live-cell imaging of RFP-Lifeact transfected hMSCs on substrates of different stiffness, recording many cells in parallel for better statistics in comparable conditions. SFs are traced with a sophisticated filament tracking program [3] and a tool to extract filament modes [4], to gain a deeper understanding of SF formation dynamics in early stem cell differentiation. This leads to a non-monotonic dependence of SF polarization on the Young's modulus of the underlying substrate[2].

[1] A. Engler et al., Cell (2006); [2] A. Zemel et al., Nature Physics (2010); [3] B. Eltzner et al., arXiv:1408.4002, 2014; [4] S. Huckemann et al., arXiv:1404.3300, 2014;

CPP 63.11 Thu 12:45 H 1028

**Elasticity of 3D networks with rigid filaments and compliant crosslinks** — •Knut M. Heidemann[1], Abhinav Sharma[2], Florian Rehfeldt[2], Christoph F. Schmidt[2], and Max Wardetzky[1] — [1]Institut für Numerische und Angewandte Mathematik, Georg-August-Universität, Göttingen — [2]Drittes Physikalisches Institut – Biophysik, Georg-August-Universität, Göttingen

Disordered filamentous networks with compliant crosslinks exhibit a low linear elastic shear modulus at small strains, but stiffen dramatically at high strains. Experiments have shown that the elastic modulus can increase by up to three orders of magnitude while the networks withstand relatively large stresses without rupturing. Here, we perform an analytical and numerical study on model networks in three dimensions. Our model consists of a collection of randomly oriented rigid filaments connected by flexible crosslinks that are modeled as wormlike chains. Under the assumption of affine deformations in the limit of *infinite* crosslink density, we show analytically that the nonlinear elastic regime in 1- and 2-dimensional networks is characterized by power-law scaling of the elastic modulus with the stress. In contrast, 3-dimensional networks show an exponential dependence of the modulus on stress. Independent of dimensionality, if the crosslink density is *finite*, we show that the only persistent scaling exponent is that of the single wormlike chain. Consequently, unlike suggested in prior work, the model system studied here cannot provide an explanation for the experimentally observed linear scaling of the modulus with the stress in filamentous networks.

# CPP 64: Flow-Induced Structures in Complex Fluids (with DRG, Deutsche Rheologische Gesellschaft, and DY)

Time: Thursday 9:30–12:00 Location: C 264

CPP 64.1 Thu 9:30 C 264

**Rheology of PMMA solutions - the role of maximum stretch ratio in the nonlinear regime** — •Sara L. Wingstrand[1], Qian Huan[1], Nicolas J. Alvares[2], and Ole Hassager[1] — [1]Technical University of Denmark, Kgs Lyngby, Denmark — [2]Drexel University, Philadelphia, USA

This work concerns linear and nonlinear rheology of poly(methyl methacrylate) (PMMA) solutions. Oligomeric methyl methacrylate is used as solvent. The concentration of polymer in solution has been adjusted, such that the maximum stretch ratio ($\lambda_{max}$) is equal to that of a polystyrene melt of 285 kg/mol (PS-285k). Accordingly, the molar mass of PMMA has been selected to obtain the same number of entanglements (Z) as the PS-285k. The solutions are characterized both in small amplitude oscillatory shear and in uniaxial extension, where the influence of $\lambda_{max}$ and Z is investigated. It is found that the linear behavior of the PMMA solutions obey the tube model with a dilution exponent of 1. Consequently, as intended, the normalized dynamic moduli of the solutions overlap those of PS-285k. In the nonlinear regime the PMMA solutions exhibit a greater resemblance with PS-285k, than other polymers having same Z but significantly different values of $\lambda_{max}$. Nevertheless, the observed trend in extensional steady state viscosity vs. strain rate differs. Consequently we conclude that introducing $\lambda_{max}$ in the tube model to enable application in the nonlinear regime, is not sufficient for obtaining a unifying model valid for polymer melts and solutions together.

CPP 64.2 Thu 9:45 C 264

**Linear and Nonlinear Rheological Behavior of Carboxymethyl Hydroxypropyl Guar Gum** — •Daniel Szopinski[1], Ulrich A. Handge[2], Werner-Michael Kulicke[1], Volker Abetz[2,3], and Gerrit A. Luinstra[1] — [1]Institute of Technical and Macromolecular Chemistry, University of Hamburg, Hamburg, Germany — [2]Institute of Polymer Research, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — [3]Institute of Physical Chemistry, University of Hamburg, Hamburg, Germany

Guar gum is a natural non-ionic polysaccharide from the endosperm of the guar bean (cyamopsis tetragonoloba), which primarily grows in India and Pakistan. The water-thickening property is the main driver for its industrial application, which is resulting from the high molecular weight (1000-2000 kg/mol) and the formation of superstructures. Guar gum may be chemically modified with carboxymethyl (CM) and/or hydroxypropyl (HP) entities to enhance the thermal stability and solubility in water. A comprehensive rheological characterization of carboxymethyl hydroxypropyl guar gum (CMHPG) will be presented. Material functions were determined in experiments under steady state shear flow, small amplitude oscillatory shear flow (SAOS) and extensional flow (CaBER). The flow behavior at the application relevant nonlinear viscoelastic region was mapped in large amplitude oscillatory shear (LAOS) experiments. Structure-property relationships were established for dilute and more concentrated solutions as function of concentration and molecular weight. It is a basis for a description of the superstructures that guar gum and its derivatives form in water.

CPP 64.3 Thu 10:00 C 264

**Relation between rheological and GPC triple detection characterization of photo-oxidated LDPE** — •Víctor Hugo Rolón-Garrido, Matthias Kruse, and Manfred H. Wagner — Chair of Polymer Engineering/Polymer Physics Berlin Institute of Technology (TU Berlin), Fasanenstr. 90, D-10623, Berlin

Sheets of low-density polyethylene (LDPE) were subjected to photo-oxidation in the presence of air using a xenon lamp to irradiate the samples for times between 1 day and 6 weeks. The formation of long-chain branching up to 1 week of degradation and the competition between chain scission and crosslinking at longer periods of radiation were investigated by rheological characterization, Fourier transform infrared spectroscopy, and the solvent extraction method (Rolón-Garrido and Wagner. Polym Degrad Stabil 2014, 99:136, Rolón-Garrido and Wagner. J Rheol 2014, 58:199). The same samples are studied here by size exclusion chromatographic characterization using triple detection (concentration, light scattering and viscosity). The results are correlated with the model parameters (beta and f2max) of the MSF model. It is confirmed that the parameter beta correlates with the gel content, while f2max is found to correlate with the experimentally determined contraction factors. By comparing the data of this study with those obtained earlier for polystyrene comb melts with well defined structure, the influence of the branching frequency on f2max becomes evident.

CPP 64.4 Thu 10:15 C 264

**Relaxation Mechanism and Molecular Structure Study of Polymer Blends by Rheological and SANS experiments** — •Ludovica Hengeller[1], Qian Huang[1], Nicolas J. Alvarez[2], Andriy Dorokhin[1], Jacob Kirkensgaard[3], Kristoffer Almdal[1], Kell Mortensen[3], and Ole Hassager[1] — [1]Technical University of Denmark, Kgs. Lyngby, Denmark — [2]Drexel University,Philadelphia, USA — [3]Copenhagen University

Industrial polymers are largely polydisperse systems. One step towards understanding polydisperse polymers is the characterization of bi-disperse blends. Even though linear viscoelastic properties of bi-disperse polystyrene blends have been investigated thoroughly both theoretically and experimentally in recent years, both nonlinear shear and extensional flow properties are lacking. The purpose of the present study is to investigate the nature of interactions, namely polymer-polymer, in strong elongational flow using a bi-disperse polystyrene blend of 95 K and 545 K Mw with 50% weight ratio. We present both uniaxial extension and stress relaxation experiments to determine if orientation and extension of long PS chains induce orientation and extension in shorter chains. The extensional viscosity of systems investigated, provides only indirect evidence about the extent to which the molecules have been unraveled and stretched by the flow field. More directed information is obtained by neutron scattering on quenched liquid bridges of polystyrene. The results of such experiments will be discussed.

CPP 64.5 Thu 10:30 C 264

**Flow-induced crystallisation of polylactides** — •Dietmar Auhl, Nils Leone, Yogesh Deshmukh, and Sanjay Rastogi — Maastricht University, Maastricht, The Netherlands

Polylactides (PLA) obey like many biopolymers a relatively poor crystallisation behaviour and are therefore difficult to process. In addition, PLA grades may vary in D,L-enantiomer distribution and form a stereocomplex, which significantly affects the crystallisation as well as final properties or product performance. Therefore, various routes are employed to control and improve the formation of crystal domains further to optimisation of processing conditions, e.g. chain modifications, addition of plasticisers or nucleating agents [1]. In this study, the crystallisation behaviour and morphology of such different PLA grades has been investigated in detail by rheo-microscopy with polarised light imaging as well as rheo-scattering for a broad range of thermo-mechanical histories and superposed to calorimetric data from thermal analysis. The comparison of experiments and molecular theory both highlight the flow-induced effects on polymer chains of initially equilibrated Gaussian conformation that enhance the crystallisation process, for which the total deformation and rate in relation to the time scales of molecular motions are decisive. [1] Saeidlou, S.; Huneault, M. A.; Li, H.; Park, C. B. Prog. Polym. Sci. (2012) 1657.

**15 min. break**

CPP 64.6 Thu 11:00 C 264

**Rheological and SEC characterization of long-chain branched poly(ethylene terephthalate)** — •Matthias Kruse, Víctor Hugo Rolón Garrido, and Manfred H. Wagner — Chair of Polymer Engineering/Polymer Physics, Berlin Institute of Technology (Berlin), Fasanenstrasse 90, D-10623 Berlin, Germany

Reactive processing is an effective and economic method to produce customized polymers fulfilling improved or additional properties. We report on reactive extrusion of poly(ethylene terephthalate) (PET) and demonstrate that linear PET can be converted into long-chain branched (LCB) PET via chain extension thereby broadening the range of possible applications. An anhydride and an epoxy based chain extender were employed, which react with the functional end groups of linear PET. Different concentrations of the two tetrafunctional coupling reagents were used to achieve different degrees of branching and to compensate for the degradation of the polymer during extrusion. The formation of LCB was proven by dynamic plate-plate rheometry and leads to a more pronounced shear thinning behavior and an increase in the complex viscosity. The increase of molecular weight and polydispersity are also confirmed by size exclusion chromatography using triple detection (concentration, light scattering and viscosity). The elongational viscosity measurements conducted with a SER device show an unexpected influence of the chain extender on the type of sample rupture at larger extensions, and give clear evidence of different levels of strain hardening with respect to the chain extender content, as quantified by the molecular stress function (MSF) model.

CPP 64.7 Thu 11:15 C 264

**Foaming of polystyrene-block-poly(4-vinyl pyridine) diblock copolymers: Thermal, rheological and processing properties** — Maria Schulze[1], •Ulrich Alexander Handge[1], Jelena Lillepärg[1], Sofia Rangou[1], and Volker Abetz[1,2] — [1]Institute of Polymer Research, Helmholtz-Zentrum Geesthacht, Max-Planck-Straße 1, 21502 Geesthacht, Germany — [2]Institute of Physical Chemistry, University of Hamburg, Grindelallee 117, 20146 Hamburg, Germany

Because of the high demand of polymer foams for application in the fields of lightweight construction, membrane technology, thermal and acoustic isolation the characterization of thermal and rheological properties of polymers for foam extrusion processes is of high relevance. In this study, we discuss the thermal and rheological properties of polystyrene-b-poly(4-vinyl pyridine) diblock copolymers and processing of these diblock copolymers via batch foaming. Carbon dioxide is used as blowing agent. High pressure differential calorimetry measurements reveal that the solution of carbon dioxide in these diblock copolymers leads to a decrease of the glass transition temperature of the polystyrene and the poly(4-vinyl pyridine) blocks. Furthermore rheological experiments in the oscillatory mode were carried out in order to elucidate the influence of composition and molecular weight on the flow properties. Stress-growth experiments reveal that the steady-state viscosity is characterized by a pronounced structure viscous behavior. Batch foaming experiments show that a larger molecular weight yields a lower foam density.

CPP 64.8 Thu 11:30 C 264

**Combined rheology and structure analysis techniques** — •Jörg Läuger — Anton Paar Germany, Ostfildern, Germany

The simultaneous use of rheological and structural analysis techniques is helpful to gain a better understanding of the dependencies between the microstructure and the mechanical properties of complex fluids. Optical techniques like Small-Angle-Light-Scattering (SALS) or microscopy measurements have been used in combination with rheology. Other techniques are Small-Angle-X-ray (SAXS) and Neutron (SANS) Scattering. The decision on which technique to choose is based on the size and type of the structure as well as on the general sample properties to be investigated. Density and orientation fluctuations within a sample, averaged over the whole scattering volume, can be well monitored by SALS. The advantage that individual structure elements are seen in microscopy can be turned into a disadvantage when combined with a rheometer. At larger shear rates or deformations the specific structure element easily moves out of the field of view and can*t be followed during an experiment. A way to overcome this issue is the use of a rheometer employing two motors operating in a counter rotation or counter oscillation fashion. The aim of this paper is to give an overview over the various techniques used for structural investigations simultaneous to rheological measurements and to introduce some new techniques and methods.

CPP 64.9 Thu 11:45 C 264

**Combined rheo-optics and rheo-scattering study of structure evolution in biobased liquid-crystalline polymers** — •Dietmar Auhl[1], Carolus Wilsens[1], Eric Stellamanns[2], and Sanjay Rastogi[1] — [1]Maastricht University, Maastricht, The Netherlands — [2]Photon Science DESY, Hamburg, Germany

Thermotropic liquid-crystalline polymers (TLCP) are often used in high-performance applications, for which the chemical composition and flow effects on the micro- and mesoscale orientation need to be well designed. Recently developed TLCP based on p-hydroxybenzoic acid, suberic acid, and vanillic acid are partially aliphatic in contrast to commercial TLCP such as ”Vectra”, and they exhibit stable nematic melt morphologies up to 300°C [1,2]. In this study, we investigate the effects of temperature, shear deformation and rate on the molecular orientation and relaxation by rheo-optics as well as rheo-scattering with x-ray and small-angle light-scattering. The results show that the threaded morphology on a mesoscale breaks and orients along the flow direction under continuous flow, while also the molecules orient on a microscopic scale. The study provides detailed insights into the structure evolution of TLCP and a unique toolbox to correlate molecular parameters to properties and performance. [1] Wilsens, C., Noordover, B., Rastogi, S. Polym. (2014) 2432; [2] Wilsens, C., Verhoeven, J., Noordover, B., Hansen, M., Auhl, D., Rastogi, S. (2014) 3306

## CPP 65: (Hydro)gels and Elastomers

Time: Thursday 9:30–10:30 Location: PC 203

CPP 65.1 Thu 9:30 PC 203

**Application of a micro-structure based model to filler reinforced elastomer compounds typically used for rubber rollers** — •Jan Plagge and Manfred Klüppel — Deutsches Institut für Kautschuktechnologie e.V., Hannover, Germany

The mechanical properties of several typical rubber roller compounds are investigated to get a deeper insight into the aging and wear mechanisms of rubber rollers under praxis conditions. For this purpose, a micro-structure based theoretical model is used linking the macroscopic mechanical response to microscopic network parameters, among them polymer-network moduli, polymer-filler-bond strengths and average filler-cluster-size. This so-called Dynamic Flocculation Model (DFM) is based on the non-affine tube model for highly entangled polymer networks and additionally takes into account hydrodynamic amplification by filler clusters as well as cyclic cluster-breakage and re-aggregation of filler-filler bonds. The influence of cross-linker-type and -concentration on the network parameters is investigated. Additionally, the effect of thermal aging is studied, whereby the focus is put on the polymer-filler and filler-filler bonds. To establish a connection to macroscopic quantities, several mechanical tests, including tensile strength, rebound and hardness are carried out for different stages of aging and cross-linker concentration. It can be concluded that the DFM is a very promising approach to relate aging and wear to changes in the microscopic structure of the polymer-filler-network.

CPP 65.2 Thu 9:45 PC 203

**Excluded volume effects in polymer brushes at moderate chain stretching** — •Dirk Romeis and Michael Lang — Leibniz-Institut für Polymerforschung Dresden e.V.

We develop a strong stretching approximation for a polymer brush made of self-avoiding polymer chains [1]. The density profile of the brush and the distribution of the end monomer positions in stretching direction are computed and compared with simulation data. We find that our approach leads to a clearly better approximation as compared to previous approaches based upon Gaussian elasticity at low grafting densities (moderate chain stretching), for which corrections due to finite extensibility can be ignored. Ref. [1] Romeis, D.; Lang, M.; Journal of Chemical Physics 141 (10) 104902 (2014)

CPP 65.3 Thu 10:00 PC 203

**Tunable microcavities with dielectric elastomer actuators** — •Irma Slowik[1], Nils Kronenberg[3], Markus Franke[2], Hartmut Fröb[1], Malte Gather[3], Andreas Richter[2], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, TU Dresden, Deutschland — [2]Institut für Halbleiter- und Mikrosystemtechnik, TU Dresden, Deutschland — [3]School of Physics, University of St Andrews, Scotland

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. 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 excellent potential for tunable optical elements like tunable phase plates, cavities, or gratings.

We discuss the design and performance of an electrically tunable multi-half wavelength cavity. Here, the cavity resonance can be tuned by changing the cavity thickness due to electrostriction of the soft elastomer. For a proof of principle, metal-elastomer-DBR cavities are build, which exhibit quality factors between 100 and 800. Applying a voltage between a bottom ITO electrode and the top metal layer leads to a reversible shift of the cavity modes up to 15 nm, which relates to a cavity thickness change of about 400 nm. Depending on the metal film thickness, the Young's modulus of the device differes between 10-300 kPa.

CPP 65.4 Thu 10:15 PC 203

**Biomimetic adhesives with self-healing properties** — •Weina Wang[1,2], Yisheng Xu[1], Xuhong Guo[1], and Regine von Klitzing[2] — [1]State Key Laboratory of Chemical Engineering, East China University of Science and Technology, Shanghai, People's Republic of China — [2]Physikalische Chemie, TU Berlin, Straße des 17. Juni 124, 10623 Berlin, Germany

Marine mussels live in the harsh seawater environment by attaching themselves onto any hard surface due to the functional unit, DOPA, in their adhesive proteins. To copy this adhesive property into synthetic material, Dopa was grafted onto poly(acrylicacid) (PAA) backbone.

In our work, the highest ratio of DOPA in mussel was mimicked into the biomimetic material PAA-DOPA. Taking advantage of a weak divalent ion, a tunable crosslinking method from reversible to irreversible was obtained. The crosslinked bioadhesive possesses water-endurable adhesion and self-healing properties by increasing pH value in sequence. The optimization of the cohesive and adhesive forces imparts the material with both hardness and adhesive properties. Besides, this adhesive is injectable and could be cured near body temperature effectively. Such properties make it the ideal candidate as wound sealant in tissue engineering process.

## CPP 66: Low-Dimensional Systems: Molecular Conductors (joint session with CPP, HL, MA, O)

Time: Thursday 9:30–11:00 Location: H 3010

CPP 66.1 Thu 9:30 H 3010

**Nature of the empty electronic states of TCNQ and their thermal evolution due to the CDW instability of TTF-TCNQ revealed by NEXAFS** — •Alisa Chernenkaya[1], K. Medjanik[1,2], P. Nagel[3], M. Merz[3], S. Schuppler[3], E. Canadell[4], J.-P. Pouget[5], and G. Schönhense[1] — [1]JGU, Mainz, Germany — [2]MAX-lab, Lund, Sweden — [3]KIT, Karlsruhe, Germany — [4]ICMAB, Bellaterra, Spain — [5]Uni Paris-Sud, Orsay, France

The electronic structure of TTF-TCNQ was studied by near-edge x-ray absorption fine structure (NEXAFS) to detect a signature of the Peierls transition at 54 K [1]. All experimental unoccupied TCNQ orbitals predicted by first-principles calculations are clearly resolved, the $\sigma^*(\pi(\mathrm{a}_g,\ \mathrm{b}_3u))$ orbital was observed for the first time [2]. The temperature dependence of NEXAFS peak intensities gives evidence of a subtle modification of the electronic structure when the charge density wave (CDW) fluctuations develop as the Peierls transition of the TCNQ stacks is approached from higher temperatures. These changes are explained on the basis of the charge transfer, the shape of the lower empty TCNQ molecular orbitals and the deformation of TCNQ during the pre-transitional CDW fluctuations. Finally the data suggest that the internal stack deformation consisting in a substantial out of plane displacement of the central ring with respect to the cyano-groups allows to gain C-C bonding energy which helps the stabilization of the Peierls transition on the TCNQ stack.

[1] J.P. Pouget, Z. Kristallogr. 219, 711, 2004.
[2] A. Chernenkaya et al., EPJB, accepted.

CPP 66.2 Thu 9:45 H 3010

**Observation of charge localization and the charge ordering transition in $(\mathbf{TMTTF})_2\mathbf{AsF}_6$ using NEXAFS** — •Katerina Medjanik[1], Alisa Chernenkaya[2], Sergej Nepijko[2], Gunnar Öhrwall[1], Pascale Foury-Leylekian[3], Pere Alemany[4], Enric Canadell[5], Gerd Schönhense[2], and Jean-Paul Pouget[3] — [1]Lund University, MAX IV Laboratory, 22100 Lund, Sweden — [2]Institut für Physik, JOGU, 55099 Mainz, Germany — [3]Laboratoire de Laboratoire de Physique des Solides, Université Paris-Sud, 91405 Orsay, France — [4]IQTCUB, Universitat de Barcelona, 08028 Barcelona, Spain — [5]ICMAB-CSIC, 08193 Bellaterra, Spain

High-resolution near-edge X-ray absorption fine structure (NEXAFS) measurements at MAX II, Lund (beamline I1011 [1]) were performed on a $(\mathrm{TMTTF})_2\mathrm{AsF}_6$ [2] single crystal upon cooling from room temperature to 90 K. Systematic shifts of different spectral features of the F 1s and S 2p signal by up to 0.8 eV to opposite sides on the photon-energy scale with respect to the spectra at room temperature have been detected. Most likely, the shift of the S 2p signal is connected with the breakdown of itinerant conductivity and loss of screening when entering the charge-localization regime.The appearance of a new F 1s pre-edge signal upon entry into the charge ordering (CO) phase at 90 K is a clear fingerprint of the reorganization of the anions in the layered material and changing in the dimerization of molecular orbitals with respect to room temperature.Project funded by DFG through SFB Transregio 49.

[1] I. A. Kowalik et al., J. Phys.: Conf. Ser. 211, 012030 (2010);
[2] M. de Souza et al., Physica B, 405, 92 (2010).

CPP 66.3 Thu 10:00 H 3010

**Low-Energy Excitations in the Quantum Spin Liquid $\kappa$-$(\mathbf{BEDT\text{-}TTF})_2\mathbf{Cu}_2(\mathbf{CN})_3$** — •Andrej Pustogow[1], Elena Zhukova[2], Boris Gorshunov[2], Marko Pinteric[3,4], Silvia Tomic[4], John Schlueter[5], and Martin Dressel[1] — [1]1. Physikalisches Institut Universität Stuttgart — [2]Moscow Institute of Physics and Technology, Russia — [3]Faculty of Civil Engineering, Maribor, Slovenia — [4]Institut za fiziku, Zagreb, Croatia — [5]Argonne National Laboratory, USA

The suppression of long range magnetic order due to geometrical frustration gives rise to the quantum spin liquid state. Theoretical considerations predict enhanced absorption within the Mott gap caused by spinons, which results in a low-frequency power-law behaviour of the optical conductivity, i.e. for $\hbar\omega_c < J \approx 250K$. To verify this hypothesis, the optical conductivity of the spin liquid candidate $\kappa$-$(\mathrm{BEDT\text{-}TTF})_2\mathrm{Cu}_2(\mathrm{CN})_3$ was measured, where the dimerized organic molecules are arranged on a triangular lattice. An extremely wide energy range from radio frequencies up to the near infrared $(10^{-13}eV - 1eV)$ was covered by dielectric spectroscopy, THz absorption and optical reflectivity measurements. We could indeed identify a power-law behaviour $\sigma(\omega) \propto \omega^\beta$ where two distinct exponents $\beta$ change from 0.9 to 1.7 at low temperatures, with the corresponding crossover scaling with temperature: $\hbar\omega_c \approx k_BT$. While our results agree well with $(\mathrm{ZnCu})_3$ $(\mathrm{OD})_6$ $(\mathrm{Cl})_2$, another spin liquid candidate, theory predicts exponents of 2 and 3.33, respectively. Hence, these experimental findings may motivate a refinement of the theoretical framework.

CPP 66.4 Thu 10:15 H 3010

**Mott criticality in organic charge-transfer salts $\kappa$-(BEDT-TTF)$_2$X studied by thermal expansion under He-gas pressure** — •E. Gati[1], R. S. Manna[1], U. Tutsch[1], B. Wolf[1], L. Bartosch[2], T. Sasaki[3], H. Schubert[1], J. A. Schlueter[4], and M. Lang[1] — [1]Physikalisches Institut, Goethe Uni, SFB/TR49, D-60438 Frankfurt — [2]Inst. für Theoretische Physik, Goethe Uni, D-60438 FfM — [3]IMR, Tohoku University, Sendai 980577, Japan — [4]Materials Science Division, National Laboratory, Argonne, Illinois 60439, USA

The Mott transition and the underlying universality class have been intensively studied in the past. The proposal of a hitherto unknown *unconventional* universality class for the quasi 2D organic charge-transfer salt $\kappa$-$(\mathrm{BEDT\text{-}TTF})_2\mathrm{Cu}[\mathrm{N}(\mathrm{CN})_2]\mathrm{Cl}$ ($\kappa$-Cl) [1], based on resistivity measurements, has attracted particular interest. In this compound, the Mott transition can be accessed by chemical pressure or the application of very small hydrostatic pressures of 300 bar. We will present measurements of the thermal expansion of $\kappa$-Cl under $^4$He-gas pressure

[2], an unique technique, which provides a very sensitive tool to investigate critical phenomena [3,4], including effects of coupling of electrons to the crystal lattice [5]. A comparison of our results with theoretical predictions of a scaling theory [4] shows that the critical properties are incompatible with the proposed unconventional universality class.

[1] F. Kagawa et al., Nature 436, 534 (2005).
[2] R. S. Manna et al., Rev. Sci. Instrum. 83, 085111 (2012).
[3] M. de Souza et al., PRL 99, 0370031 (2007).
[4] L. Bartosch et al., PRL 104, 245701 (2010).
[5] M. Zacharias et al., PRL 109, 176401 (2012).

CPP 66.5 Thu 10:30 H 3010

**Electronic structure and superconductivity of multi-layered organic charge transfer salts** — •Harald O. Jeschke, Michaela Altmeyer, Daniel Guterding, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt

We examine the electronic properties of polymorphs of (BEDT-TTF)$_2$Ag(CF$_3$)$_4$(TCE) (1,1,2-trichloroethane) within density functional theory (DFT). While a phase with low superconducting transition temperature $T_c = 2.6$ K exhibits a $\kappa$ packing motif, two high $T_c$ phases are layered structures consisting of $\alpha'$ and $\kappa$ packed layers. We determine the electronic structures and discuss the influence of the insulating $\alpha'$ layer on the conducting $\kappa$ layer. In the $\kappa$-$\alpha'_1$ dual-layered compound, we find that the stripes of high and low charge in the $\alpha'$ layer correspond to a stripe pattern of hopping parameters in the $\kappa$ layer. Based on the different underlying Hamiltonians, we study the superconducting properties and try to explain the differences in $T_c$.

CPP 66.6 Thu 10:45 H 3010

**New Charge Transfer Systems based on PAHs** — •Antonia Morherr[1], Sebastian Witt[1], Martin Baumgarten[2], Harald O. Jeschke[3], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe Universität Frankfurt, D-60438 Frankfurt am Main — [2]MPI für Polymerforschung, D-55128 Mainz — [3]Institut für Theoretische Physik, Goethe Universität Frankfurt, D-60438 Frankfurt am Main

The Polycyclic Aromatic Hydrocarbons (PAHs) Picene, Coronene and Phenanthrene attracted strong attention in the last years as first superconducting PAHs when intercalated with potassium [1]. K$_3$Picene shows a T$_c$ of 18 K and the T$_c$ of intercalated Coronene lies between 3.5 K and 15 K [2].
Here, we present charge transfer complexes with PAHs representing donor or acceptor molecules of these complexes. The knowledge of different crystallization modes of these systems, e.g. mixed stack or alternating stack configuration, are important for the physical properties. The complexes were grown by horizontal vapor growth technique or by growth from solution. Crystal structures, electrical transport measurements and spectroscopical investigations are presented in this contribution. In addition to the experimental data, we present bandstructure calculations, which were performed by density functional methods. The interpretation of both is one approach to understand growing conditions of different stack configurations and an important step towards the design of new charge transfer complexes.

[1] R. Mitsuhashi et al., Nature 464, 76 (2010)
[2] Y. Kubozono et al., Phys. Chem. Chem. Phys. 13, 16476, (2012)

## CPP 67: Mitgliederversammlung der Deutschen Rheologischen Gesellschaft (DRG)

Time: Thursday 12:00–13:00 Location: C 264

**60 min. meeting**

## CPP 68: Focus Session Hybrid Photovoltaics and Perovskites (joint session CPP, HL)

Time: Thursday 15:00–18:15 Location: C 130

**Invited Talk** CPP 68.1 Thu 15:00 C 130

**Photophysics of organic-inorganic hybrid lead iodide perovskite single crystals** — •Maria Antonietta Loi — Zernike Institute for Advanced Materials, University of Groningen, The Netherlands

Hybrid organometal halide perovskites have been demonstrated to have outstanding performance as semiconductors for solar energy conversion. Further improvement of the efficiency and stability of these devices requires a deeper understanding of their intrinsic photophysical properties. Here we address the intrinsic material physics by investigating the structural and optical properties of high quality single crystals of Methyl Ammonium Lead Iodide from room temperature to 5K. X-ray diffraction reveals an extremely sharp transition at 163 K from a twinned tetragonal I4/mcm phase to a low-temperature phase characterized by complex twinning and possible frozen disorder. Above the transition temperature the photoluminescence is in agreement with a band-edge transition, explaining the outstanding performances of the solar cells. Whereas below the transition temperature, three different features arise, one of which is attributed to a singlet-free-exciton and the other two to bound-triplet excitons. The bound-triplet excitons are characterized by a decay dynamics of about 5$\mu$s and by a saturation phenomenon due to many-body interactions. This results in a description of the room temperature recombination as being due to spontaneous band-to-band radiative transitions and weak non-radiative Auger processes, whereas a diffusion-limited behaviour is expected for the low temperature range.

**Invited Talk** CPP 68.2 Thu 15:30 C 130

**Exciton stabilization in hybrid lead-halide perovskites: photophysical versus structural properties** — •Annamaria Petrozza — Istituto Italiano di Tecnologya, Milan, Italy

Hybrid perovskites represent a new, disruptive technology in the field of optoelectronics. Hybrid halide perovskites, e.g. CH3NH3PbX3 [X = Cl, Br, or I], are usually deposited as polycrystalline thin-films with variable mesoscale morphology depending on the growth conditions. The obtained grain size ranges from tens to thousands of nm. Over the last two years the impressive improvement of photovoltaic performance has been driven by radical empirical evolution of the device architecture and processing methodologies. However, there is a considerable lack of understanding of material properties, both as pristine films and their embodiment in a device. Here we demonstrate, through a combination of femto-second transient absorption spectroscopy, structural analysis and multi-scale modeling as a function of crystal size and temperature, that the electron-hole interaction is sensitive to the microstructure of the material. We find that by control of the material processing during fabrication both free carrier and Wannier excitonic regimes are accessible. Thus, a definitive classification excitonic or free carrier semiconductor is not possible. The long-range order of the organic cation dipole field is disrupted by polycrystalline disorder introducing domain walls where dipole twinning breaks down. The variations in electrostatic potential found for smaller crystallites suppress exciton formation, while larger crystals of the same composition demonstrate an unambiguous excitonic state.

CPP 68.3 Thu 16:00 C 130

**Morphology-dependent ultrafast spectroscopy of lead-halide perovskite for electro-optical applications** — •Simon Bretschneider, Melike Karakus, Valentin Kamm, Enrique Cánovas, and Frédéric Laquai — Max Planck Institut für Polymerforschung, Mainz

Lead-halide perovskite have emerged as a new class of materials for electro-optical, especially photovoltaic applications with power conversion efficiencies now up to 20% [1]. High-performance electro-optical devices rely on perovskite films without pinholes, flat surface and well-defined thickness. Due to the organic/inorganic nature of the lead-halide perovskite and the criticalness of a pure perovskite phase without impurities of the precursors, utilization of solution-processing is non-trivial.

The combination of time-resolved photoluminescence and transient absorption spectroscopy is a powerful tool, which allows for the investigation of generation and recombination of charge carriers in lead-halide perovskite films on a femto- to microsecond timescale and across a spectral range from Vis to NIR. In this work, we present pump-probe transient absorption measurements of solution-processed lead-halide perovskite films grown in ambient and dry nitrogen atmosphere using different post-processing annealing schemes. The findings of ultrafast spectroscopy suggest that the performance of lead-halide perovskite films for electro-optical applications relies more on homogeneous films than on specific crystal sizes.

[1]NREL Chart of record cell efficiencies (28.11.2014).

CPP 68.4 Thu 16:15 C 130

**Time-resolved confocal microscopy of hybrid metal halide perovskite thin films** — •Kathrin Bader, Richard Ciesielski, Nadja Giesbrecht, Johann M. Feckl, Irene Grill, Fabian C. Hanusch, Thomas Bein, Pablo Docampo, Matthias Handloser, and Achim Hartschuh — Department Chemie and CeNS, LMU Munich, Germany

Organic-inorganic metal halide perovskite solar cells (PSCs) have seen an unprecedented development over the past 4 years due to their potential to fulfill most requirements for large scale production. Extremely fast progress in the field of perovskite absorbers has taken solar cell efficiencies from 10 % in 2012 [1] to over 19 % in 2014 [2]. A crucial parameter for the functioning of solar cells is a long charge carrier diffusion length that allows to effectively collect photogenerated charges. To determine this diffusion length several experimental methods have been reported that either provide indirect information or use electrical contacts [3,4]. We used time-resolved laser scanning confocal microscopy to visualize the transport range and timescale of photo-excited species within the film. The experimentally observed transport length range up to several microns under high light intensity conditions. Our results help to explain the high short circuit currents that can be achieved in PSCs. Financial support by the DFG through the Nanosystems Initiative Munich (NIM) is gratefully acknowledged. [1] M. M. Lee et al., Science 338, 643 (2012) [2] H. Zhou et al., Science 345, 542 (2014) [3] S. D. Stranks et al., Science 342, 6156 (2013) [4] E. Edri et al., Nat. Commun. 5, 3461 (2014)

CPP 68.5 Thu 16:30 C 130

**Preparation and characterization of methylammonium lead halide perovskite solar cells in planar-type configuration** — •Philipp Rieder[1], Matthias Fischer[1], Stefan Väth[1], Andreas Baumann[2], Kristofer Tvingstedt[1], and Vladimir Dyakonov[1,2] — [1]Experimentelle Physik 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg — [2]Bayerisches Zentrum für Angewandte Energieforschung, 97074 Würzburg

In recent years, the use of organometal halide compounds as the photoactive layer in solar cells has attracted a lot of attention, with power conversion efficiencies (PCE) reaching up to 20.1% already. The performance and properties of this material class are strongly dependent on the crystallinity of the layer, with the working principles still being unclear and part of ongoing research. By synthesizing our own methylammoniumiodide as the organic precursor, we are able to fabricate solution processed planar heterojunction perovskite solar cells with an active layer consisting of $CH_3NH_3PbI_3$ or $CH_3NH_3PbI_{3-x}Cl_x$. PCE values of the working devices exceeding 10% under solar illumination are achieved. The crystallinity and surface quality of the films are analyzed via scanning electron microscopy, atomic force microscopy and x-ray diffraction. The solar cells are characterized by means of current-voltage measurements, external quantum efficiency and photoluminescence.

CPP 68.6 Thu 16:45 C 130

**Spatially resolved photocurrent generation in organolead halide perovskite solar cells** — Thomas J.K. Brenner, Andreas Paulke, Natalie Schön, Roberta Saponaro, and •Dieter Neher — Institute of Physics & Astronomy, University of Potsdam, Germany

Hybrid perovskite solar cells have shown to be efficient in various device structures, for example in planar, vapour deposited films, in and on mesostructured metal oxides and in solution-processed films of different crystallinity. Here, we study ITO/PEDOT:PSS/CH3NH3PbI3/PCBM/C60/BCP/Al devices with different perovskite crystallinity and identify regions of efficient photocurrent generation with submicrometer resolution. We establish a relationship between crystallinity and device performance and study the role of grain boundaries for photocurrent generation. We correlate our results to time delayed collection field (TDCF) measurements of charge generation to identify ways to further enhance photocurrent generation in this class of photovoltaic devices.

**15 min. break.**

CPP 68.7 Thu 17:15 C 130

**Unbalanced Charge Distribution Inside a Perovskite-Sensitized Solar Cell in Real Space** — •Victor W. Bergmann[1], Stefan A.L. Weber[1], F. Javier Ramos[2], Mohammad Khaja Nazeeruddin[3], Michael Grätzel[3], Dan Li[1], Anna L. Domanski[1], Ingo Lieberwirth[1], Shahzada Ahmad[2], and Rüdiger Berger[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Abengoa Research, Seville, Spain — [3]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Solar cells based on perovskite light absorbing materials reached power conversion efficiencies >20%. Today, the knowledge about the local charge generation processes inside these solar cells is limited. We prepared smooth cross sections by means of focused ion beam milling such that the full structure and functionality of the devices were preserved [1]. This way, the internal interfaces between the different materials in the cell are accessible for frequency modulation Kelvin Probe Force Microscopy (FM-KPFM). Upon illumination under short-circuit conditions, holes accumulate in front of the hole transport layer, which is proof of an unbalanced charge transport. This potential barrier reduces the charge transfer towards the electrode. Furthermore after light illumination, we measured remaining charges inside the active device area. These charges were attributed to traps in the material. In conclusion, the FM-KPFM method allows us not only to map the local contact potential variation but also to correlate it with the local structure of the functional layers.

[1] Bergmann et al. Nature Communications 5, 5001 (2014).

CPP 68.8 Thu 17:30 C 130

**Charge Transport in Dye-sensitized Solar Cells: What do J-transients really depend on?** — •Frank Marlow, Abigail Hullermann, and Lisanne Messmer — MPI für Kohlenforschung, 45470 Mülheim an der Ruhr, Germany

J-transients (electrical current transients) following a laser excitation are considered as a powerful tool for the understanding of the action of dye-sensitized solar cells. In the last years, a sophisticated model for their understanding has been established which, however, turns out to be in contradiction with a number of experimental findings including the J-signal shape and the signal dependences on experimental parameters. It is especially remarkable that there are the always delays of the electrical signal after the laser excitation and that the possible diffusion times do not follow an Einstein diffusion relation which is a-priori assumed in many works.

CPP 68.9 Thu 17:45 C 130

**Spray deposition of titania films with introduction of crystalline nanoparticles for solid-state dye-sensitized solar cells** — •Lin Song[1], Weijia Wang[1], Volker Körstgens[1], Daniel Moseguí González[1], Yuan Yao[1], Norma K. Minar[2], Dina Fattakhova-Rohlfing[2], Stephan V. Roth[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]LMU München, Department of Chemistry and Center for NanoScience, Butenandtstr.5-13 (E), 81377 Munich — [3]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany

Solid-state dye-sensitized solar cells (ssDSSCs), using solid-state hole transporting materials (HTM) as alternatives for dye generation and hole transport, have received immense attention because such photovoltaic devices avoid the leakage and corrosion problems in conventional DSSCs. In particular, ssDSSCs based on TiO2 and organic HTM are of great interest due to the combined advantages of both organic and inorganic components. We investigate this kind of solar cells fabricated using mesoporous titania films as electron transporting materials, a metal-free dye D149 as a light harvester, and P3HT as HTM. For optimizing the device performance, we introduce crystalline titania nanoparticles into the titania film in order to obtain a more effective titania photoanode. Moreover, spray coating is employed for the film deposition because it is simple, low cost, and usable for large-scale production. The morphology and crystallinity of titania films are investigated, showing a crucial influence on final device performance.

CPP 68.10 Thu 18:00 C 130

**ZnO coated TiO2 photoanodes with improved electron**

**transfer for dye sensitized solar cells** — •Bo Liu[1], Peter Lemmens[1], Andrey Bakin[2], Andreas Waag[2], Aidin Lak[3], Meinhard Schilling[3], Winfried Daum[4], and Samir Kumar Pal[5] — [1]IPKM, TU-BS, Braunschweig — [2]IHT, TU-BS, Braunschweig, Germany — [3]EMG, TU-BS, Braunschweig, Germany — [4]IEPT, TU Clausthal — [5]SNBC, Kolkata, India

ZnO coated TiO2 photoanodes for cost efficient dye sensitized solar cells are prepared using anodization of a metal electrode leading to an array of TiO2 nanotubes. Atomic layer deposition is used for the conformal covering by ZnO. Following hematoporphyrin sensitization the improved electron transfer is probed using time resolved fluorescence. Work supported by RTG-DFG 1953/1, Metrology for Complex Nanosystems and the Laboratory for Emerging Nanometrology, TU Braunschweig.

## CPP 69: Biomaterials and Biopolymers (joint session CPP, BP)

Time: Thursday 15:00–18:00 Location: C 264

CPP 69.1 Thu 15:00 C 264

**Dynamic and static force measurements on (PLL/HA)n multilayer films by atomic force microscopy** — •Johannes Hellwig and Regine von Klitzing — Stranksi-Laboratorium, TU Berlin, 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, ionic strength and temperature of the surrounding medium changes. Furthermore the viscoelastic film behaviour was measured and calculated by dynamic force measurements.

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(2) Decher, G. Science 1997, 277, 1232.

(3) Üzüm, C.; Hellwig, J.; Madaboosi, N.; Volodkin, D.; v. Klitzing, R. Beilstein J. Nanotechnol. 2012, 3, 778.

CPP 69.2 Thu 15:15 C 264

**Mechanical characterization of recombinant spider silk: yarn tensile testing and single fiber deformation via AFM** — •Benedikt Neugirg[1], Gregor Lang[2], Thomas Scheibel[2], and Andreas Fery[1] — [1]Physical Chemistry II, University of Bayreuth — [2]Biomaterials, University of Bayreuth

Outstanding mechanical properties combined with biocompatibility render spider silks one of the most promising materials with respect to biomedical applications. Recombinant routes to e.g. dragline silk core proteins of Araneus diadematus provide access to material fabrication at industrially relevant scales. Together with the electrospinning technique, morphologies based on fibrillar structures, from single fiber to nonwovens are readily producible.

In our work, we mechanically characterize recombinant silk yarns and the individual sub-um diameter fibers which the yarns consist of. For this purpose we use macroscopic tensile testing and nanoscopic AFM lateral bending experiments. Furthermore, we investigate the influence of the relative humidity (RH) which is known to have a huge impact on silk mechanics.

We found the recombinant silk to resemble rubber-like properties at higher levels of RH. Enhancing structure crystallinity by post-treatment of the fibers dramatically increases the energy uptake at high RH prior to rupture. In this (physiologically relevant) humidity range, recombinant spider silk can keep up with its natural analog in terms of toughness, the most prominent mechanical characteristic.

CPP 69.3 Thu 15:30 C 264

**Wang-Landau simulation of protein-like Gō model molecules** — •Arne Böker and Wolfgang Paul — Martin-Luther-Universität Halle-Wittenberg

The Wang-Landau method is a recent addition to the Monte Carlo family, able to provide complete thermodynamic information about a system. Contrary to Markovian Monte Carlo, it works in a generalized statistical ensemble, giving the opportunity to access quantities of microcanonical and canonical ensembles in one simulation.

Gō-like protein models have been successful for several decades owing to their simplicity, allowing fast simulation to achieve mostly reasonable results. Thus, they provide a suitable model system for the relatively complicated Wang-Landau algorithm.

We applied this method to a basic Gō model consisting of hard tangent spheres with a square-well attraction to investigate the phase behaviour and especially the influence of the length scale used to define neighbours within the Gō model on these properties.

CPP 69.4 Thu 15:45 C 264

**The effect of specific interactions on the state diagram of a hard-sphere chain model** — •Benno Werlich[1], Timur Shakirov[1], Mark Taylor[2], and Wolfgang Paul[1] — [1]Institut für Physik, Martin-Luther Universität Halle-Wittenberg, Halle(Saale), Germany — [2]Department of Physics, Hiram College, Ohio, USA

Secondary structure formation in proteins is generated by an interplay of unspecific and specific interactions. We employ a coarse-grained, one-bead protein-like model to qualitatively understand the importance of the specific interactions. Based on a hard-sphere chain model with unspecific square well attractions we introduce specific interactions as additional square well potentials. These interactions are selective and correspond to a simple donor acceptor representation in the context of hydrogen bonds. The donor acceptor interaction strength can be changed via variation of the well depth of the square well potential. A comparison between hard-sphere chains with and without specific interactions shows a strong deviation in certain ranges of the density of states (DOS). The DOS is the basic function which encodes the whole thermodynamics and thus the microcanonical and canonical analysis give a more detailed insight. To generate the DOS we applied the Stochastic Approximation Monte Carlo method.

CPP 69.5 Thu 16:00 C 264

**Characterization of a liposomal drug carrier with continuous contrast variation in SAXS** — •Raul Garcia-Diez[1], Christian Gollwitzer[1], Michael Krumrey[1], and Zoltan Varga[2] — [1]Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, 10587 Berlin, Germany — [2]Biological Nanochemistry Research Group, Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Magyar Tudosok korutja 2, H-1117, Budapest, Hungary

Doxorubicin is an anticancer drug known for its high cardiotoxicity, though a liposomal formulation of it can reduce this side-effect significantly and improve the pharmacokinetics of the drug. In this work, the mean size and average density of pegylated liposomal doxorubicin (Caelyx®) was determined by continuous contrast variation in SAXS with iodixanol, an iso-osmolar suspending medium. The study is focused on the isoscattering point position and the analysis of the Guinier region of the scattering curves recorded at different solvent densities at the four-crystal monochromator beamline of PTB at the synchrotron radiation facility BESSY II. The response of the liposome to increasing solvent osmolality and the structure of the liposome-encapsulated doxorubicin fiber after the osmotic shrinkage of the liposome are evaluated with sucrose contrast variation in SAXS/WAXS.

CPP 69.6 Thu 16:15 C 264

**Binding of amino acids to bioactive calcite surface** — •Robert Stepić[1], Zlatko Brkljača[1], David M. Smith[2,3], and Ana-Sunčana Smith[1] — [1]Institute for Theoretical Physics and Excellence Cluster: Engineering of Advanced Materials, FAU Erlangen-Nürnberg, Nägelsbachstraße 49b, Erlangen, 91052, Germany — [2]Division of Organic Chemistry and Biochemistry, Rudjer Bošković Institute, Bijenička 54, 10000, Zagreb, Croatia — [3]Center for Computational Chemistry, FAU Erlangen-Nürnberg, Nägelsbachstraße 25, Erlangen, 91052, Germany

Biomineralization is a process by which living organisms form minerals. This process is controled mainly by proteins and the resulting end products have distinctively different properties than minerals produced by abiotic mineralization. Better understanding of underlying mechanisms of biomineralization could help us make use of them in wide range of applications. Our goal is to gain further insight into the role of proteins in biomineralization by taking their elementary building blocks, amino acids, and investigating their interactions with a calcite surface in water. To achieve this we use a well established theoretical framework of molecular dynamics implemented in free GROMACS package. Efficient sampling of the phase space is done using the harmonic bias potential along the suitable reaction coordinate. This allows us to construct the potential of mean force and determine the free energies of binding to the surface of various amino acids. Results of this research will give us clues as to what amino acids play a key role in proteins that control the process of biomineralization.

**15 min. break**

CPP 69.7 Thu 16:45 C 264

**Investigation of the lateral arrangement of phospholipid monolayers with respect to the adsorption of hyaluronan*** — •Florian Wieland[1], Thomas Zander[1], Sören Gayer[1], Andra Dedinaite[2], Per Claesson[2], Vasyl Haramus[1], and Regine Willumeit-Römer[1] — [1]Helmholtz Zentrum Geesthacht, Max Planck Str. 1, 21502 Geesthacht — [2]KTH Royal Institute of Technology, School of Chemical Sciences and Engineering, Department of Chemistry, Surface and Corrosion Science, Drottning Kristinas väg 51, SE-10044 Stockholm, Sweden

The unmatched tribological performance of articulated joints is due to both the properties of the cartilage itself and the assumed self-organization of the molecules in the synovial fluid and at the surface of cartilage. Phospholipids form lamellar structures on cartilage surfaces and are able to reduce friction and wear. We performed x-ray reflectivity and grazing incidence diffraction measurements on Langmuir layers of Dipalmitoylphosphatidylcholine and investigated how the adsorption of hyaluronan (HA) changes the arrangement of the lipids. In the course of the experiment we changed parameters like the molecular weight (MW) and the salt concentration in the subphase, in order to determine the key parameters.

Our data indicate that the adsorption strongly depends on the MW of HA and further on the presence of divalent ions in the subphase.

CPP 69.8 Thu 17:00 C 264

**Interaction of Hyaluron and Phospholipids at high hydrostatic pressure** — •Thomas Zander[1], Florian Wieland[1], Min Wang[2], Akanksha Raj[2], Per Claesson[2,3], Andra Dedinaite[2,3], Vasyl Haramus[1], Regine Willumeit-Römer[1], and Andreas Schreyer[1] — [1]Helmholtz Zentrum Geesthacht, Institute for Materials Research, DE-21502 Geesthacht — [2]KTH Royal Institute of Technology, School of Chemical Sciences and Engineering, SE-10044 Stockholm — [3]SP Technical Research Institute of Sweden, SP Chemistry, SE-11486 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 keep 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.

X-ray reflectivity measurements at different hydrostatic pressures (60bar - 2kbar) on silicon supported phospholipid- and phospholipid hyaluronen composite layers have been performed in order to gain information about their structural arrangement. Parameters like, temperature, molecular weight of the hyaluronan and ions in the solvent solution have been varied, to identify possible key parameters for good lubrication. Our results clearly reveal differences in the behaviour of the phospholipid hyaluronen composites due to different solvent conditions.

CPP 69.9 Thu 17:15 C 264

**Establishing Short-Range Gradients of Cytokines to Mimic Paracrine Cell Interactions in vitro** — •Michael Ansorge and Tilo Pompe — Universität Leipzig, Institute of Biochemistry

Cells in various tissues receive myriads of exogenous signals, which in sum determine their fate. Many signaling molecules act in a gradient fashion to guide cell migration, differentiation and proliferation. We set up a microparticle-based system for generating biomimetic short-ranged gradients to analyze dynamic cell behavior with high resolution in vitro. The modification of agarose microbeads with glycosaminoglycans (GAG) with different degree of sulfation provides a toolbox to tune the binding and release of various cytokines.

Using chemically sulfated hyaluronic acid (HA) as GAG we were able to load the microbeads with different cytokines (SDF-1, TGF-beta, IL10) in dependence on their affinity to sulfated and non-sulfated HA. By following the local concentration decrease of fluorescently labeled cytokine inside the microbeads over days with confocal microscopy we could determine released amounts and diffusion-based transport properties. We were able to calculate local cytokine gradients surrounding the microbeads, which are estimated to be in the range of some tens of micrometers at physiological concentrations of pg/ml. We currently verify these local gradients using fluorescence correlation spectroscopy.

Studies on the dynamic cell behavior within the cytokines gradients address biomedical questions on cell fate of hematopoietic stem cells and fibroblasts in 3D collagen-based matrices.

CPP 69.10 Thu 17:30 C 264

**Characterising the water vapour sorption behaviour of wood** — •Alexander Murr and Roman Lackner — Institut for Structural Engineering and Material Science, University of Innsbruck

Wood is a cellular material with a hierarchical structure based on polymers (cellulose, hemicelluose and lignin). As variations of humidity causes a change of its physical properties, a detailed knowledge of the interaction between water and wood is of importance. A common method for such investigations are water vapour sorption (wvs) experiments where relative humidity is varied and the related change of sample mass is measured. As this change of mass deviates from classical diffusion, various macroscopic models appeared in literature, ranging from relaxation limited to transport limited approaches. To identify which of these descriptions could be used for further investigations, a precise identification of the macroscopic behaviour is necessary.

In the given presentation the sorption kinetics of Norway spruce wood (Picea abies) will be discussed. Based on a series of wvs experiments on grained wood the influence of grain size and temperature on the sorption behaviour will be shown. A comparison of similar sample masses with different grain sizes illustrates diffusion along the cell wall not being the limiting factor in the observed sorption experiments. Additionally, an outlook on further theoretical and experimental investigations shall be given.

CPP 69.11 Thu 17:45 C 264

**Kinetics of mutarotation in fucose-saccharides as monitored by dielectric and infrared spectroscopy** — •Wilhelm Kossack[1], Wycliffe Kiprop Kipnusu[1], Mateusz Dulski[2], Karolina Adrjanowicz[2], Olga Madejczyk[2], Emanuel Urandu Mapesa[1], Martin Tress[1], Kamil Kaminski[2], and Friedrich Kremer[1] — [1]University of Leipzig, Linnestr. 5, Leipzig, Germany — [2]University of Silesia, Katowice, Poland

Fourier Transform Infrared Spectroscopy and Broadband Dielectric Spectroscopy are combined to trace kinetics of mutarotation in L-fucose. After quenching molten samples to temperatures between $T = 313$ K and 328 K, the concentrations of two anomeric species change according to a simple exponential time dependence, as seen by the increasing absorbance of specific IR-vibrations. In contrast, the dielectric spectra reveal a slowing down of the structural ($\alpha$-) relaxation according to a stretched exponential time dependence (stretching exponent of $1.5 \pm 0.2$). The rates of change in the IR absorption for $\alpha$- and $\beta$-fucopyranose are (at $T = 313$ K) nearly one decade faster than that of the intermolecular interactions as measured by the shift of the $\alpha$-relaxation. This reflects the fact that the $\alpha$-relaxation monitors the equilibration at a mesoscopic length scale, resulting from fluctuations in the anomeric composition.

## CPP 70: Complex Fluids and Soft Matter - Part III (joint session DY, CPP, BP)

Time: Thursday 15:00–16:45 Location: BH-N 334

**Invited Talk** CPP 70.1 Thu 15:00 BH-N 334

**Melting of soft disks: From liquid-hexatic coexistence to continuous transitions** — •Sebastian C. Kapfer[1,2], Manon Michel[2], and Werner Krauth[2] — [1]Theoretische Physik 1, FAU Erlangen, Germany — [2]LPS, Ecole normale supérieure, Paris, France

The melting transition of two-dimensional solids has been a subject of continued research for more than fifty years, with the prevalent scenarios being the KTHNY theory of defect unbindung and a conventional first-order liquid-solid transition. For hard disks, the KTHNY scenario has recently been essentially confirmed, even though the liquid-hexatic step is of first order [1]. Using a new rejection-free global-balance Monte Carlo algorithm [2], we show that this result transfers to soft interactions with inverse power-law or Yukawa potentials [3]. The order of the liquid-hexatic step can be tuned from first-order to continuous by softening the potential. We show that there is always a hexatic phase separating the liquid and solid phases, and identify two regimes of the hexatic with vastly different correlation lengths. These results rationalize a plethora of simulation results obtained in the past, and could be verified in charged-colloid experiments.

[1] E. P. Bernard, W. Krauth, Phys. Rev. Lett. 107, 155704 (2011).
[2] M. Michel, S. C. Kapfer and W. Krauth, JCP 140, 054116 (2014).
[3] S. C. Kapfer, W. Krauth, preprint at arXiv:1406.7224.

CPP 70.2 Thu 15:30 BH-N 334

**Quasicrystalline Order and a “Crystal-Liquid" State in a Soft-Core Fluid** — •Andrew Archer[1], Alastair Rucklidge[2], and Edgar Knobloch[3] — [1]Department of Mathematical Sciences, Loughborough University, Loughborough, LE11 3TU, UK — [2]Department of Applied Mathematics, University of Leeds, Leeds LS2 9JT, UK — [3]Department of Physics, University of California at Berkeley, Berkeley, CA 94720, USA

Results will be presented for a two-dimensional system of soft particles interacting via a two-length-scale potential that may be considered to be a simple model for the effective interaction between dendrimers and other such polymeric macromolecules in solution. Density functional theory and Brownian dynamics simulations reveal the system has a fluid phase and two crystalline phases with different lattice spacing. Of these the larger lattice spacing phase can form an exotic periodic state with a sizeable fraction of highly mobile particles: a “crystal liquid”. Near the transition between this phase and the smaller lattice spacing phase, quasicrystalline (QC) structures may be created by a competition between linear instability at one scale and nonlinear selection of the other. This dynamic mechanism for forming QCs is qualitatively different from mechanisms observed previously. The system first forms a small length scale crystal. Only when this phase is almost fully formed (i.e., the dynamics is far into the nonlinear regime) does the longer length scale start to appear, leading to the formation of QCs [A.J. Archer, A.M. Rucklidge, and E. Knobloch, Phys. Rev. Lett. **111**, 165501 (2013)].

CPP 70.3 Thu 15:45 BH-N 334

**A New Particle-Based Mesoscopic Model for Nematic Liquid Crystals** — •Kuang-Wu Lee and Marco G. Mazza — Max-Planck-Institut für Dynamik und Selbstorganisation, 37077 Gottingen, Germany

We introduce a new mesoscopic model for nematic liquid crystals (LCs). This approach combines the particle-based stochastic rotation dynamics (SRD) method and the Ericksen-Leslie formulation of nematohydrodynamics. SRD has been used to investigate hydrodynamics at the mesoscopic level because it recovers the Navier-Stokes equation. We extend the SRD scheme to anisotropic fluids, i.e. nematic liquid crystals, by including the Ericksen-Leslie equations. We verify the applicability of this hybrid model by few study-cases in LC physics, e.g. the temperature-driven isotropic-nematic phase transition and the rheology of sheared LC. Our simulation results show that this hybrid model captures many essential aspects of LC physics at the macroscopic scale, while preserving microscopic thermal fluctuations.

CPP 70.4 Thu 16:00 BH-N 334

**Molecular simulations of liquid crystalline ferrofluids** — •Stavros Peroukidis and Sabine Klapp — Institute of theoretical physics, Technical University of Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We explore the phase behavior and self assembly in binary mixtures of uniaxial rod and magnetic dipolar sphere particles by means of molecular simulations. We find that the mesogenic rods support the formation of orientational ordered ferromagnetic chains which, in turn, enhance the order of the liquid crystal. This ends up to liquid crystalline ferrofluids that possess two principal directors (one for each species). The antiparallel arrangement of the ferromagnetic chains, within the mesophases, cancels out macroscopic spontaneous magnetization. Depending on the relative size of the species, the directors are on average either parallel or perpendicular to each other, giving rise to uniaxial or biaxial liquid crystalline ferrofluids including: nematic, smectic, columnar phases and phase transformations between them.

CPP 70.5 Thu 16:15 BH-N 334

**Density functional theory for elongated polyhedra** — •Matthieu Marechal and Klaus Mecke — Friedrich-Alexander-Universit\"at Erlangen-N\"urnberg

Due to recent advances in synthesis of nanoparticles and colloids, many-particle system of polyhedra are readily available for experiments. This has spurred a host of many-particle simulation studies on polyhedra. Recently, the lack of theoretical tools to study these system was amended by proposing a density functional theory (DFT) for polyhedra using the frame work of fundamental measure theory.

In this contribution, the application of DFT to elongated polyhedra will be discussed. Recent advancements in the DFT of long rods allow us to consider nematic and smectic liquid crystals in addition to the isotropic phase. We will consider these phases for triangular prisms that are elongated along their rotational symmetry axes. Colloids with this shape could be synthesized using nanolithography. We calculate the liquid crystal phase diagram and compare our results to Monte Carlo simulations.

CPP 70.6 Thu 16:30 BH-N 334

**Dynamical Crossover at the Liquid-Liquid Transformation of a Compressed Molten Alkali Metal** — Taras Bryk[1,2], Simone De Panfilis[3,1], Federico A Gorelli[4,5], Eugene Gregoryanz[6], Michael Krisch[7], Giancarlo Ruocco[1,5], Mario Santoro[8], Tullio Scopigno[1,5], and •Ari Paavo Seitsonen[9,10] — [1]Dip. Fisica, Univ. La Sapienza, Roma, Italy — [2]Inst. Cond. Matter Phys. of NASU, Lviv, Ukraine — [3]Centre for Life Nano Science IIT@Sapienza, Istituto Italiano di Tecnologia, Roma, Italy — [4]Eur. Lab. for Non-Linear Spectr., Firenze, Italy — [5]IPCF-CNR, c/o Univ. La Sapienza, Italy — [6]Centre for Science at Extreme Conditions, Univ. Edinburgh, United Kingdom — [7]Eur. Synchr. Res. Facility, Grenoble, France — [8]IFAC-CNR, Sesto Fiorentino, Italy — [9]Dept. Chemie, Univ. Zürich, Switzerland — [10]Dépt. Chimie, ENS Paris, France

Density-driven phase transformations are a known phenomenon in liquids. Pressure-driven transitions from an open low-density to a higher-density close-packed structure were observed for a number of systems. Here, we show a less intuitive, inverse behavior. We investigated the electronic, atomic, and dynamic structures of liquid Rb along an isothermal line at 573 K, at 1.2-27.4 GPa, by means of ab initio molecular dynamics simulations and inelastic x-ray scattering experiments. Above 12.5 GPa, the breakdown of the nearly-free-electron model drives a transition of the pure liquid metal towards a less metallic, denser liquid, whose first coordination shell is less compact. Our study unveils the interplay between electronic, structural, and dynamic degrees of freedom along this liquid-liquid phase transition.

# CPP 71: Glasses and Glass transition (joint session DY, CPP, DF)

Time: Thursday 15:00–17:30 Location: BH-N 128

CPP 71.1 Thu 15:00 BH-N 128

**Binary colloidal mixtures investigated by differential dynamic microscopy** — •Tatjana Sentjabrskaja, Marco Laurati, and Stefan U. Egelhaaf — Condensed Matter Physics Laboratory, Heinrich-Heine University, D-40225 Duesseldorf, Germany

We investigate dynamics of colloids in binary mixtures of hard spheres with large size asymmetry, using confocal differential dynamic microscopy (con-DDM). This technique allows to study wave vector dependent dynamics of particles by analysing time series of confocal microscopy images. Analysis of the Fourier spectra of image differences acquired at different delay times allows to determine the time-dependent density-density correlation functions and, from its shape and decay time, the nature and characteristic times of particles' dynamics. To benchmark con-DDM, we investigate one-component systems of colloidal particles at different volume fractions. Diffusion coefficients of particles as a function of volume fraction obtained from con-DDM measurements are found to be in good agreement with those obtained using dynamic light scattering experiments. We additionally show that con-DDM can be used to separately study the dynamics of single species in multicomponent systems using fluorescent labeling. In particular, we are able to determine the dynamics of sub-resolution tracer particles in binary colloidal mixtures with large size asymmetry, as a function of increasing volume fraction of the large particles. The motion of the tracer, small particles becomes increasingly constrained by the dense matrix of large spheres, resulting in complex, non-diffusive motion of the tracers.

CPP 71.2 Thu 15:15 BH-N 128

**Critical-like behaviour in non-crystalline solids caused by angular correlations** — •Mariya Rasshchupkyna[1,2,3], Volodymyr Bugaev[3,4], Johannes Roth[5], Gerhard Grübel[6,1], and Peter Wochner[3,4] — [1]The Hamburg Centre for Ultrafast Imaging (CUI) — [2]University of Hamburg — [3]Max Planck Institute for Intelligent Systems, Stuttgart — [4]Max Planck Institute for Solid State Research, Stuttgart — [5]Institute for Functional Materials and Quantum Technologies, University of Stuttgart — [6]DESY

Modern experimental techniques on the basis of coherent scattering data, such as X-ray cross-correlation analysis (XCCA) [1] allow the direct determination of angular correlations (and their modes) in molecular disordered systems. We performed molecular dynamics (MD) simulations for model systems with Dzugutov-type [2] interaction adjusted for the creation of glassy-type quasi-equilibrium states. XCCA applied to the simulated coherent scattering patterns of the MD samples reveals a four-point dodecagonal dominant mode responsible for the formation of non-commensurate structures, as found in glasses and quasicrystals. Strikingly, this mode exhibits a pronounced temperature-dependence indicating a critical-type behavior in the vicinity of the glassy-type transition.

References

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2. M. Dzugutov, Phys. Rev. Lett. 70, 2924 (1993).

CPP 71.3 Thu 15:30 BH-N 128

**Nonaffine deformations, glass transition, and yielding in disordered solids** — •Alessio Zaccone — Physics-Department, Technische Universität München

A new approach to the glass transition has been recently developed from the angle of nonaffine elasticity. Due to structural disorder, the particle motions in glasses under shear do not merely follow the imposed affine pathways prescribed by the strain tensor of standard continuum linear elasticity, but deviate significantly to undergo additional nonaffine displacements. Importantly, these nearest-neighbour forces would exactly cancel out mutually in any ordered lattice with local center-inversion symmetry. The concept of nonaffine free energy of deformation can be applied to molecular and atomic glasses. The resulting scheme has been implemented to predict the T-dependence of the shear modulus of polymer glasses and its vanishing at the glass transition. The main effect leading to vanishing of rigidity can be identified with the decrease of the average effective intermolecular connectivity as the material expands upon increasing T. In turn, this makes the negative nonaffine contribution to free energy become increasingly more important as T rises, until the free energy of deformation vanishes at a critical temperature for mechanical instability, which is very close to the calorimetric glass transition. Besides nonaffinity, an important role is played by anharmonic interactions which control the thermal expansion coefficient of the glass, which in turn controls how connectivity decreases with increasing T.

CPP 71.4 Thu 15:45 BH-N 128

**The Potential Energy Landscape of microrheologically driven supercooled liquids** — •Carsten F. E. Schroer[1,2] and Andreas Heuer[1,2] — [1]Westfälische Wilhelms-Universität, Münster, Germany — [2]NRW Graduate School of Chemistry, Münster, Germany

We perform computer simulations of a fragile model glass-former in which a single particle is driven by an external force through the liquid. Thereby, we track the path the system takes through its underlying Potential Energy Landscape (PEL) and aim for understanding how this is altered by the external field[1,2] and how the altering is related to the nonlinear responses of dynamic quantities.

In the PEL approach, the dynamics of undriven (strong *and* fragile) glass formers have found to be very well described in terms of an improved trap model, the Gaussian Glass Former (GGF)[3]. In this talk we want to demonstrate, how the GGF can be extended to driven supercooled liquids. This enables one to predict typical nonlinear responses like the nonlinear decay of the local friction coefficient as well as highly nontrivial effects like the occurrence of effective temperatures. Within this framework we can quantitatively predict the numerically observed effective temperatures in terms of the kinetics of the force-dependent hopping processes in the PEL. This establishes an intimate relation between the thermodynamics and the kinetics also in the highly non-equilibrium regime.

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[3] A. Heuer, *J. Phys.: Condens. Matter* **20**, 373101 (2008)

CPP 71.5 Thu 16:00 BH-N 128

**Physical mechanisms of nonlinear conductivity: A model analysis** — •Andreas Heuer and Lars Lühning — Institute for Physical Chemistry, University of Münster, Germany

Nonlinear effects are omnipresent in thin films of ion conducting materials showing up as a significant increase of the conductivity upon increasing electric field. For a disordered hopping model general physical mechanisms are identified giving rise to the occurrence of positive or negative nonlinear effects, respectively. Analytical results are obtained in the limit of high but finite dimensions [1]. They are compared with the numerical results for 3D up to 6D systems. A very good agreement can be found. The results can also be used to rationalize previous numerical simulations. The implications for the interpretation of nonlinear conductivity experiments on inorganic ion conductors are discussed.

[1] A. Heuer, L. Lühning, J. Chem. Phys. 140, 094508 (2014).

**15 min. break**

CPP 71.6 Thu 16:30 BH-N 128

**Where to go in a rough free-energy landscape?** — •Stefan Schnabel and Wolfhard Janke — Universität Leipzig

Frustrated spin systems like the Edwards-Anderson spin glass are notorious for disorder-induced frustration. Sampling their rough free-energy landscape is very challenging and only small systems can be investigated. Over the years great efforts have been made to improve both hardware and implementation, yet the basic method for the investigation of 3d spin glasses is and has been parallel tempering [1]. Here, we explore the possibility of using additional information obtained by a local minimization procedure similar to the basin-hopping algorithm [2]. Altering the statistical weight of conformations according to the depth of nearby local minima can reduce autocorrelation time. We investigate whether this improvement outweighs the additional computational cost.

[1] K. Hukushima and K. Nemoto, J. Phys. Soc. Japan 65 (1996) 1604. [2] D. J. Wales, J. Phys. Chem. A 101 (1997) 5111.

CPP 71.7 Thu 16:45 BH-N 128

**Evidence for a Novel Relaxation Mechanism in Glasses at Very Low Temperatures** — •Marius Hempel, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, 69120 Heidelberg

The acoustic and dielectric properties of amorphous solids at low temperatures are governed by two level tunneling systems and can be described in similar ways. One difference is however, that electric fields couple only to tunneling systems carrying an electric dipole moment, whereas acoustic measurements couple to all tunneling systems. Thus, the two methods complement each other and can therefore lead to a better understanding of the underlying processes.

Low frequency measurements of the dielectric properties of the two multicomponent glasses N-KZFS11 and HY-1, containing significant amounts of tantalum and holmium respectively, have recently shown unexpected behavior, which cannot be understood in terms of the so called standard tunneling model. This behavior has been attributed to the very large nuclear electric quadrupole moments of $^{181}$Ta and $^{165}$Ho.

We present the first measurements of the acoustic properties of N-KZFS11 and HY-1 in the kHz range down to 10 mK. The results of these measurements underpin the observations seen in dielectric experiments and provide further evidence for a novel relaxation mechanism in such glasses.

CPP 71.8 Thu 17:00 BH-N 128

**Non-Universal Dielectric Properties of Glasses at Very Low Temperatures** — •Annina Luck, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, 69120 Heidelberg

The universal behaviour of amorphous solids at low temperatures, governed by two level tunneling systems and described by the standard tunneling model, has long been a generally accepted fact. In the last years, however, measurements of dielectric two-pulse polarization echoes have revealed that nuclear electric quadrupole moments involved in atomic tunneling systems can cause specific material-dependent effects in magnetic fields.

We show measurements of dielectric properties of the two multicomponent glasses N-KZFS11 and HY-1, containing significant amounts of tantalum and holmium respectively. As $^{181}$Ta and $^{165}$Ho both carry very large nuclear electric quadrupole moments, these glasses are ideal candidates to determine the influence of these moments on the physical properties of glasses down to very low temperatures.

Our measurements not only show unique dielectric behaviour in both glasses, but also differ significantly from various predictions of the standard tunneling model.

CPP 71.9 Thu 17:15 BH-N 128

**Thermography on Luminescent Barium Borate Glass for White-LED Applications** — •Florian Wagner[1], Peter Nolte[2], and Stefan Schweizer[1,2] — [1]South Westphalia University of Applied Sciences, Lübecker Ring 2, 59494 Soest — [2]Fraunhofer Application Center for Inorganic Phosphors, Branch Lab of Fraunhofer Institute for Mechanics of Materials IWM, Lübecker Ring 2, 59494 Soest

White light-emitting diodes (W-LEDs) represent one of the most promising lighting technologies for the future. Primarily used in many lighting applications is a blue LED combined with a yellow phosphor. The phosphor powder is usually embedded in an organic polymer and coated onto the LED chip. Heat-induced degradation of the organic encapsulate, however, results in an efficiency decrease and color temperature change. Luminescent glasses or glass ceramics are an interesting alternative due to their higher thermal and chemical stability. This work focuses on the thermal behaviour of luminescent barium borate glasses under intense excitation with ultraviolet/blue light. The glasses are doped with rare-earth ions for optical activation. Upon absorbing the ultaviolet/blue light, the rare-earth ions show their typical emission in the visible spectral range. Here, not all of the absorbed light is frequency-downshifted, but a significant part is released in the form of heat. Contact-free infrared thermography enables an analysis of the heat development in these materials. An algorithm based on the partial differential heat equation is developed to calculate the heat source density of the optical excitation from the surface temperature distribution.

## CPP 72: Microswimmers, Active Liquids I (joint session CPP, BP, DY)

Time: Thursday 15:45–18:00 Location: PC 203

**Invited Talk** CPP 72.1 Thu 15:45 PC 203

**Flagellar synchronisation through direct hydrodynamic interactions** — •Marco Polin[1], Douglas Brumley[2], Kirsty Wan[3], and Raymond Goldstein[3] — [1]University of Warwick, Coventry. UK — [2]MIT, Boston, MA. US — [3]University of Cambridge, Cambridge. UK

Microscale fluid flows generated by ensembles of beating eukaryotic flagella are crucial to fundamental processes such as development, motility and sensing. Despite significant experimental and theoretical progress, the underlying physical mechanisms behind this striking coordination remain unclear. We describe a novel series of experiments in which the flagellar dynamics of two micropipette-held somatic cells of Volvox carteri, with measurably different intrinsic beating frequencies, are studied by high-speed imaging as a function of their mutual separation and orientation. From analysis of beating time series, we find that the interflagellar coupling, which is constrained by the lack of chemical and mechanical connections between the cells to be purely hydrodynamical, exhibits a spatial dependence that is consistent with theoretical predictions. At close spacings it produces robust synchrony which can prevail for thousands of flagellar beats, while at increasing separations this synchrony is systematically degraded by stochastic processes. Through dynamic flagellar tracking we quantify the associated waveforms and show that they are significantly different in the synchronised state. This study unequivocally reveals that flagella coupled only through a fluid medium are capable of exhibiting robust synchrony despite significant differences in their intrinsic properties.

**Invited Talk** CPP 72.2 Thu 16:15 PC 203

**Active motion: From single microswimmers to their emergent collective behavior** — •Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin

Active motion of artificial and biological microswimmers is relevant in microfluidics and biological applications but also poses fundamental questions in nonequilibrium statistical physics. Mechanisms of single microswimmers need to be understood and a detailed modeling of microorganisms helps to explore their complex cell design and their behavior. The collective motion of microswimmers generates appealing dynamic patterns.

In this talk I review some of our work modeling biological microswimmers such as *E. coli* [1] and the African trypanosome [2], the causative agent of the sleeping sickness, in order to contribute to their better understanding. Using simpler model microswimmers such as active Brownian particles, I will demonstrate their emerging collective behavior. Hydrodynamic interactions lead to a clustering transition dependent on swimmer type [3] or to the formation of fluid pumps in 3D harmonic traps [4]. Self-phoretic active colloids show biomimetic autochemotactic behavior, which can induce dynamic clustering, oscillating clusters, or a chemotactic collaps [5].

[1] R. Vogel and H. Stark, Phys. Rev. Lett. **110**, 158104 (2013).
[2] D. Alizadehrad et al., to be published in PLoS Comp. Biol.
[3] A. Zöttl and H. Stark, Phys. Rev. Lett. **112**, 118101 (2014).
[4] M. Hennes et al., Phys. Rev. Lett. **112**, 238104 (2014).
[5] O. Pohl and H. Stark, Phys. Rev. Lett. **112**, 238303 (2014).

CPP 72.3 Thu 16:45 PC 203

**Collective behavior and clustering of self-propelled rod shaped catalytic motors: A theoretical study** — •Davoud Pouladsaz[1] and Zahra Eskandari[2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute for Intelligent Systems, Stuttgart, Germany

In the last few years, catalytic micro-motors have attracted considerable attention and different experiments have performed in order to investigate their applicability in biology, e.g. colloidal cargo transportation. The collective behaviour of these micro-engines and their dynamic self-organization have recently been studied in experiments.

In our study, we did Brownian dynamics simulation of rigid rods as a model for the interaction of catalytic motors, in a framework of stochastic processes which explain the force generating chemical reactions, and theoretically investigated the effect of spatial geometry of these active rods in the pattern formation of their clusters.

CPP 72.4 Thu 17:00 PC 203

**Vortex pattern formation of curved active polymers** — •Lorenz Huber, Jonas Denk, Emanuel Reithmann, and Erwin Frey — Ludwig-Maximilians-Universität, München, Deutschland

During bacterial cytokinesis FtsZ filaments assemble into a ring-like structure. Recent experiments with reconstituted FtsA-dependent recruitment of FtsZ filaments to supported membranes have observed self-organization into vortex patterns. Accounting for the treadmilling dynamics of curved FtsZ on the membrane, we propose a model for systems of polymers with equal length and curvature that undergo effective propulsion. The FtsZ filaments are assumed to sterically repel each other. Employing Brownian dynamics simulations and a kinetic Boltzmann ansatz to study these systems on microscopic and mesoscopic length scales, respectively, we identify activity, intrinsic curvature, and steric repulsion as sufficient to control the stability of vortex patterns. In our microscopic approach we modeled the FtsZ membrane dynamics as a two-dimensional system of propelled elastic polymers and find a parameter regime of dense and stable vortices. Furthermore, we employed a mesoscale description in terms of a kinetic Boltzmann approach to investigate general effects of intrinsic curvature on collective behavior in active systems. We obtain a phase diagram featuring a confined parameter region of steady dense swirls. Our results provide a generic and robust mechanism for pattern formation in actual biological systems of curved filaments.

CPP 72.5 Thu 17:15 PC 203

**The many faces of drag in micro-swimming** — •Jayant Pande[1], Laura Merchant[1,2], Jens Harting[3], and Ana-S. Smith[1,4] — [1]Inst. for Theo. Phys., Friedrich-Alexander Univ., Erlangen, Germany — [2]School of Phys. and Astronomy, Univ. of St. Andrews, Scotland — [3]Dept. of Appl. Phys., Eindhoven Univ. of Technology, Eindhoven, the Netherlands — [4]Ruđer Bošković Inst., Zagreb, Croatia

Although the theoretical study of micro-swimming is becoming increasingly important, the role of the drag force faced by swimmers–clearly one of the cornerstones of micro-locomotion–remains inadequately understood. We shed light in this talk on some of the fundamental ways in which this force affects micro-swimming, using a very simple yet versatile model of a bead-spring swimmer, based on the three-sphere design of Najafi and Golestanian. The drag force on these swimmers enters in various guises–through the influence of the mean bead shape, through any induced transitory shape changes during the swimming cycle if the beads are non-rigid, and through the fluid viscosity. We consider the effect of each contribution separately by letting the beads be of any shape as well as of rigid or flexible material, and by analyzing the various forces on them in fluid. We show that in general an increase in the drag force can have a net positive or a negative impact on the velocity, and it is the swimmer elasticity which decides this. Depending on the latter, we present precise expressions for the parameter ranges where the drag has opposing effects. We support the theory using lattice Boltzmann method-based simulations, and discuss the parts of the theoretical parameter space which are accessible to the simulations.

CPP 72.6 Thu 17:30 PC 203

**Formation, compression and surface melting of colloidal clusters by active particles** — •Felix Kümmel[1], Parmida Shabestari[1], and Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universität Stuttgart, D-70569 Stuttgart, Germany — [2]Max-Planck-Institut für Intelligente Systeme, D-70569 Stuttgart, Germany

Artificial active swimmers, i.e. Janus particles, suspended in a critical binary mixture, are capable of a self-diffusiophoretic motion upon illumination [1][2]. In previous experiments, the dynamics of such swimmers close to walls and periodic arrays of rigid obstacles has been investigated [1]. Here, we experimentally examine the structural changes in a mixture of passive and a small number of active colloidal particles of equal diameters in a two-dimensional system. With increasing passive particle area fraction, we observe the formation of clusters with passive particles in the interior and active particles at their boundaries. Further increase of the passive area fraction leads to the merging and compression of such clusters and eventually to local melting of crystalline regions by enclosed microswimmers. Our results demonstrate that the addition of only a small amount of active particles largely changes the structure and the dynamics of colloidal suspensions.

[1] VOLPE G, BUTTINONI I, VOGT D, KÜMMERER H J AND BECHINGER C 2011 MICROSWIMMERS IN PATTERNED ENVIRONMENTS SOFT MATTER 7, 8810 (2011) [2] B. TEN HAGEN, F. KÜMMEL, R. WITTKOWSKI, D. TAKAGI, H. LÖWEN, AND C. BECHINGER, NATURE COMMUNICATIONS 5 (2014)

CPP 72.7 Thu 17:45 PC 203

**Detention times of microswimmers close to surfaces** — •Andreas Zöttl[1], Konstantin Schaar[1,2,3], and Holger Stark[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin — [2]Robert Koch-Institut, D-13353 Berlin — [3]Institut für Theoretische Biologie, Humoldt Universität Berlin, D-10115 Berlin

The locomotion of biological microswimmers such as bacteria in aqueous environments is determined by low-Reynolds-number hydrodynamics and influenced by thermal and intrinsic biological noise. In many relevant environments such as in the human body or in the ocean microorganisms swim in the presence of soft or solid boundaries. When bacteria approach surfaces they accumulate there and form aggregates such as biofilms. A key ingredient for the observed near-wall accumulation are the relatively large times the microswimmers reside at a surface before leaving the surface. Recently, the role of noise compared to hydrodynamic interaction with the surface for the dynamics of microswimmers at a surface has been discussed controversially.

In our work we study theoretically the collision of microswimmers with surfaces by including both hydrodynamic interactions and noise. We introduce a general framework to calculate their wall detention time distribution, i.e., the time they stay at the surface. We map the escape of the microswimmer from the surface to a mean-first passage problem and apply our theory to different swimmer models (pusher, puller, source-dipole swimmer). While source dipole swimmers have a reduced and pullers an increased detention time compared to a simple active Brownian particle, pushers can have both.

## CPP 73: Focus: Disordered Systems/Glasses under Shear (joint session CPP, DY)

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

**Invited Talk** CPP 73.1 Thu 15:30 C 243

**Microscopic flows of complex suspensions** — •Anke Lindner — PMMH-ESPCI, Paris

The flow of complex suspensions is ubiquitous in nature and industrial applications. Their non-Newtonian character is due to flow-induced orientation, rearrangement, or deformation of microscopic objects suspended in simple fluids. These objects can be isotropic or anisotropic, rigid or deformable, active or passive. Linking the microstructure on the particle level to the macroscopic response under flow is one of the fundamental scientific challenges of soft matter physics. Recent microfabrication techniques lead to a precise control of even complex particle properties and new microfluidic rheometers show high resolution. Using these new approaches, we present two examples of flows of complex suspensions in chosen microfluidic geometries which allow this link to be established. First, we use a solution of flexible polymers, where normal stresses are known to arise when the polymers are stretched under flow and characterize the onset of elastic flow instability in a serpentine channel as a function of its curvature. The calibrated serpentine channel can then be used as a sensitive rheometer to detect even small normal stresses in unknown suspensions. Second, we employ a Y-channel, a powerful rheometer for measuring shear viscosities, to study the viscosity of active suspensions of e-coli bacteria. In this way we link the activity of the bacteria to the measured non-Newtonian effective viscosity.

CPP 73.2 Thu 16:00 C 243

**Thinning and Thickening in Active Microrheology** — •Ting

Wang and Matthias Sperl — Institut für Materialphysik im Weltraum, DLR, Köln, Germany

When pulling a probe particle in a driven granular system with constant velocity, one can characterize the probe by a velocity-dependent friction coefficient. With increasing control velocity, the friction of the probe keeps constant in the small-velocity regime (linear response), decreases in the moderate-velocity regime (thinning), and then increases in the large-velocity regime (thickening).

There are three distinct processes behind those phenomena: diffusion, damping and direct collision; the magnitude of the pulling velocity determines which process dominates, resulting in thinning or thickening behavior. We confirm this physics picture by stochastic simulation.

CPP 73.3 Thu 16:15 C 243

**Transition to flow of binary glasses under applied stress or strain rate** — •Marco Laurati[1], Tatjana Sentjabrskaja[1], Jan Hendricks[1], Alan R Jacobs[2], George Petekidis[2], and Stefan U Egelhaaf[1] — [1]Condensed Matter Physics Laboratory, Heinrich-Heine University Düsseldorf — [2]IESL-FORTH, University of Crete

We investigate and compare the transition to flow of glasses composed by two species of colloidal hard spheres presenting large size asymmetry, upon application of a constant stress or constant shear rate. The transition to flow of the binary glasses is affected by the composition of the mixture, and reflects changes in the prevailing caging mechanism, i.e. transitions between different glass states [1]. Furthermore, the timescales characterising the onset of flow significantly differ depending on the nature of the applied field, i.e. stress or strain. The relaxation of the accumulated stress after removal of the applied field demonstrates the presence of residual stresses that can be tuned through the mixture's composition. The recovery of strain after creep reveals a non monotonic dependence of the recovery time as a function of the previously applied stress, with a maximum recovery time observed in correspondence to the yield stress of the glass. [1] T. Sentjabrskaja et al. (2014), Soft Matter, 10, 6546-6555.

CPP 73.4 Thu 16:30 C 243

**Yielding in concentrated colloidal dispersions: relation between stress overshoot and microscopic structure and dynamics** — Marco Laurati, Kevin Mutch, and •Stefan Egelhaaf — Condensed Matter Physics Laboratory, Heinrich Heine University, 40225 Düsseldorf, Germany

The microscopic structure and dynamics of concentrated colloidal dispersions at different times after application of shear is determined using confocal microscopy. When the stress overshoot occurs in the rheological response, we observe super-diffusion and a maximally deformed cage, i.e. maximum structural anisotropy [1,2]. The anisotropy is not only characterized by a quadrupolar (angular momentum $l = 2$) distortion expected by continuum elasticity theory, but also a higher order hexadecupolar ($l = 4$) mode which marks the transition form reversible elastic to irreversible plastic deformation [3]. This mode suggests that yielding of local cages proceeds through the rearrangement of particles in the first neighbour shells, which switch from the compressional to the extensional axis. Also in the steady-state of shear, cage-breaking events are found to persist. In addition to the anisotropic cage deformation, yielding is also accompanied by a strong rise in the isotropic ($l = 0$) distortion, which corresponds to a pressure increase.

[1] N. Koumakis et al. (2012) Phys. Rev. Lett. 108, 098303. [2] K.J. Mutch et al. (2013) Eur. Phys. J. - Special Topics 222, 2803. [3] C.P. Amann et al. (2013) arxiv:1302.2030.

CPP 73.5 Thu 16:45 C 243

**Continuum Mechanics Simulations in Glass Forming Liquids** — •Heliana Cardenas and Thomas Voigtmann — Deutsches Zentrum für Luft- und Raumfahrt, Köln, Germany

Amorphous glassy materials show complex flow features when they are formed by solidification of dense liquids. An important feature of such systems is the non-linear nature of the flow rule relating stresses and strains when they are perturbed by external forces. The transition itself is characterized by slow dynamics where the intrinsic relaxation time plays a determining role on describing this behavior.

Schematically, the interaction of non-linear rheology and slow relaxation can be captured by so-called "fluidity" models, where the (spatially local) structural relaxation rate is a function of flow rate. The spatial dynamics of fluidity is controlled by a diffusion coefficient related to a cooperativity length scale.

We use finite volume method (FVM) to combine the resulting constitutive equation with the Navier-Stokes equations to effectively describe the flow behavior of glass-forming systems in various geometries and for different time-dependent protocols.

## CPP 74: Friction and Lubrication

Time: Thursday 17:00–17:45 Location: C 243

**Invited Talk** CPP 74.1 Thu 17:00 C 243

**Multiscale Contact Mechanics for Rough Surfaces with Applications to Rubber Friction and the Leak-rate of Rubber Seals** — •Bo Persson — FZ Juelich, Germany

Surface roughness has a big influence on the dry or lubricated contact between solids in stationary or sliding contact. Surface roughness often occurs over many decades in length scale, e.g., from nm to the linear size of the objects, which makes it a hard problem for numerical (e.g., finite element) methods. I have developed an analytical contact mechanics theory which can take into account all relevant length scales. The theory is very flexible and can be applied not only to homogeneous elastic solids but can include layering, plasticity and viscoelasticity (which is important for rubber-like materials). Both dry and lubricated contact mechanics, with or without adhesion, can be studied using this approach. The theory predicts the area of real contact, the distribution of contact stresses and the distribution of interfacial separations which is important for the leak-rate of seals or for microbial ingress during the shelf life of syringes. It also predicts the viscoelastic contribution to rubber friction and can be used to obtain the Stribeck curves for lubricated contacts. In this presentation I will describe the theory in some detail and give some applications to rubber friction and the leak-rate of rubber seals. See also www.MultiscaleConsulting.com for more information and relevant publications.

CPP 74.2 Thu 17:30 C 243

**Motion of drops on slippery surfaces** — •Frank Schellenberger, Doris Vollmer, and Hans-Jürgen Butt — Max Planck Institute for Polymer Research, Mainz, Germany

Liquid repellent, antibiofouling, pressure-stable and self-repairing surfaces would have enormous impact in industrial and medical applications. Slippery lubricant infused textured surfaces may open up novel possibilities. When a liquid drop is deposited on a slippery surface, the drop is found to slip by tilting the surface a few degrees. With the drop, dirt or also bacteria can be removed.

We used Laser Scanning Confocal Microscopy (LSCM) to observe the behavior of drops of different liquids on a lubricant infused textured surface. As textured surface we used micropillar arrays and inverse opals to hold different lubricants.

We investigated the shape of the wetting ridge surrounding a drop, the three phase contact lines, and how a drop advances and recedes on slippery surfaces. Single pinning and depinning events are resolved with micrometer and millisecond resolution. Even, cloaking of the drop is visible by using LSCM. Confocal microscopy revealed that drops on slippery surfaces have a high contact angle, typically exceeding 150°.

We expect that this understanding of the stationary and dynamic behavior or drop on slippery lubricant infused surfaces will help to design stable slippery lubricant infused surfaces.

## CPP 75: Physics of Food (joint session CPP, BP)

Time: Thursday 18:00–18:30 Location: C 264

CPP 75.1 Thu 18:00 C 264

**Small-angle scattering study on the structure of the lecithin stabilizer layer in tetracosane-water nanoemulsions and -suspensions** — •Martin Schmiele and Tobias Unruh — Physik Department, Friedrich-Alexander-Universität Erlangen–Nürnberg, Staudtstr. 3, 91058 Erlangen, Germany

Tetracosane ($C_{24}$, TCS) o/w nanoemulsions stabilized by the lecithin 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC) were prepared by high-pressure melt homogenization. The droplets (diameters of about 65 nm as measured by photon correlation spectroscopy) exhibit a strong super-cooling ($\Delta T$ about 20 K) and crystallize in a for TCS unusual orthorhombic crystal structure (space group $Pca2_1$ as verified by wide-angle x-ray scattering).

Using small-angle x-ray and neutron scattering and nanodispersions with different neutron scattering contrasts for the TCS core and the DMPC stabilizer layer, the molecular arrangement of DMPC in the interfacial layer was studied. For the nanoemulsions a dense monolayer of DMPC with a thickness of about 16.2 Å was found with only a minor interpenetration between TCS and the acyl chains of DMPC. For the nanosuspensions a monolayer thickness of 10.5 Å is found, indicating a more flat arrangement of the DMPC molecules at the interface. This could be explained by the expanded surface of the nanocrystals with respect to the emulsion droplets.

The structure of the interfacial stabilizer layer of lipid emulsions and suspensions is highly relevant with regard to lipid oxidation of bioactive compounds in food and the crystallization of nanoemulsions.

CPP 75.2 Thu 18:15 C 264

**Lipid migration in multicomponent food products such as chocolate** — •Svenja Reinke[1], Stephan V. Roth[2], Gonzalo Santoro[2], Josélio Vieira[3], Stefan Palzer[4], and Stefan Heinrich[1] — [1]Hamburg University of Technology, Denickestr. 15, 21073 Hamburg, Germany — [2]DESY, Notkestr. 85, 22607 Hamburg, Germany — [3]Nestlé Product Technology Centre York, P.O. Box 204, Haxby Road, York YO91 1XY, United Kingdom — [4]Nestlé SA, Avenue Nestlé 55, 1800 Vevey, Switzerland

Our aim is to obtain a deeper understanding of the preferred pathways of lipid molecule migration in multicomponent food materials. A profound understanding of the mechanisms is the basis for controlling undesired fat migration leading to degradation of the material quality, e.g. fat blooming of chocolate, resulting in large sales losses for the food industry. Synchrotron X-ray tomography revealed voids in an industrial chocolate sample, which are considered as having a strong impact on the plausible migration pathways. In addition, oil migration into particles with cocoa butter, which resulted in structural changes, were tracked using spatially resolved small angle X-ray scattering (SAXS). Oil migration has been observed in artificial pores produced in cocoa butter matrices with embedded particles and the analysis of wetting properties of the material has provided further insights into the migration mechanism. Although we have not yet elucidated the exact migration mechanism, our results suggest that migration could occur through the pores of the material. Future research will further clarify the role of the porous structure in chocolate fat blooming.

## CPP 76: Organic Electronics and Photovoltaics: Devices (joint session CPP, HL, TT)

Time: Friday 9:30–12:00 Location: C 130

**Invited Talk** CPP 76.1 Fri 9:30 C 130

**Strong and switchable magnetic couplings in molecular semiconductor films** — •Michele Serri[1], Wei Wu[1,2], Luke Fleet[1], Cyrus Hirjibehedin[2], Nicholas Harrison[1], Chris Kay[2], Andrew Fisher[2], Gabriel Aeppli[2], and Sandrine Heutz[1] — [1]London Centre for Nanotechnology, Imperial College London, UK — [2]London Centre for Nanotechnology, University College London, UK

Polyaromatic molecular thin films are well established as alternative semiconductors, but their magnetic properties have received less attention. This presentation will focus on phthalocyanines (Pc), archetypal molecular semiconductors that can ligate spin-bearing transition metals at their centre. They can be processed as thin films and nanowires [1] from the vapour phase and crystallise as a range of polymorphs. This leads to the formation of spin chains, and may give rise to magnetic exchange whose sign and magnitude depends on the nature of the transition metal and crystal structure [2]. A recent milestone was reached by CoPc, which exhibits antiferromagnetic coupling, with an exchange energy reaching 100 K [3]. This interaction is up to two orders of magnitude larger than in other first-row transition metal Pcs and can be obtained on flexible plastic substrates.

[1] Wang et al. ACS Nano 4 (2010) 3921. [2] Heutz et al. Adv. Mater. 19 (2007) 3618. [3] Serri et al. Nat. Commun. 5 (2014) 3079.

**15 min. break**

CPP 76.2 Fri 10:15 C 130

**Effects of Coulomb repulsion on conductance switching in organic molecules** — •Irina Petreska[1,2] and Gertrud Zwicknagl[1] — [1]Institut für Mathematische Physik, Technische Universität Braunschweig, 38 106 Braunschweig, Germany — [2]Faculty of Natural Sciences and Mathematics, Ss. Cyril and Methodius University, 1 000 Skopje, Republic of Macedonia

Charge transfer in phenylene ethynylene oligomers (OPEs), using realistically estimated effective model parameters from first principles is studied by a combined, ab initio and model approach. The aim of our work is to investigate the Coulomb correlation effects on conductance switching in OPEs. In the proposed model, molecular electronic system is restricted to one-level coupled to metallic leads, described by a two-site Hubbard Hamiltonian. Comparison of the current-voltage curves, obtained from rate equations, for the planar and perpendicular conformer, clearly demonstrates enhancement of the switching process due to two-particle correlations.

CPP 76.3 Fri 10:30 C 130

**Enhanced performance of polymeric electron injection layers for OLEDs by the use of a solvent-additive.** — •Sebastian Stolz[1,5], Martin Petzoldt[2,5], Naresh Kotadiya[1,5], Eric Mankel[3,5], Manuel Hamburger[2,5], Uli Lemmer[1,4], Norman Mechau[1,5], and Gerardo Hernandez-Sosa[1,5] — [1]Karlsruhe Institute of Technology, Light Technology Institute — [2]University of Heidelberg, Institute of Organic Chemistry — [3]Technische Universität Darmstadt, Materials Science Institute, Surface Science Division — [4]Karlsruhe Institute of Technology, Institute of Microstructure Technology — [5]InnovationLab GmbH, Heidelberg

In this work, we investigate an amino-functionalized polyfluorene as electron injection layer in OLEDs. We demonstrate that its performance can be considerably increased by adding a functionalized alkane to the polyfluorene solution. X-ray photoelectron spectroscopy shows that the polymer thickness decreases with increasing additive concentration which indicates a better packing of the polymers. At the same time, Ultraviolet photoelectron spectroscopy revals that the cathode work-function decreases with increasing additive concentration. Finally, we solution process OLEDs that use a PPV derivative commonly known as Super-Yellow as emitting layer and the polyfluorene in combination with silver as cathode layer. OLEDs, that use a mixture of functionalized alkane and polyfluorene, exhibit an about 0.8 eV lower turn-on voltage while the maximum luminance is almost doubled compared to OLEDs without additive. Furthermore, operational lifetimes are improved by a factor of two.

CPP 76.4 Fri 10:45 C 130

**Modeling of organic semiconductors: from molecular to device properties** — Pascal Kordt[1], Mustapha Al Helwi[2,3], Wolfgang Kowalsky[3], Falk May[4], Alexander Badinski[5], Christian Lennartz[4], and •Denis Andrienko[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]BASF SE, GVE/M-B009, 67056 Ludwigshafen, Germany — [3]IHF Institut, Technische Universität Braunschweig, Brunswick, Ger-

many — [4]BASF SE, GVE/M-B009, 67056 Ludwigshafen, Germany — [5]BASF SE, GVM/S-B009, 67056 Ludwigshafen, Germany

We review the progress in modeling of charge transport in disordered organic semiconductors on various length-scales, from atomistic to macroscopic. This includes evaluation of charge transfer rates from first principles, parametrization of coarse-grained lattice and off-lattice models, and solving the master and drift-diffusion equations. Special attention is paid to linking the length-scales and improving the efficiency of the methods. All techniques are illustrated on an amorphous organic semiconductor, DPBIC, a hole conductor and electron blocker used in state of the art organic light emitting diodes (OLEDs). The outlined multiscale scheme can be used to predict OLED properties without fitting parameters, starting from chemical structures of compounds.

CPP 76.5 Fri 11:00 C 130

**Combined electrical and optical analysis of the efficiency roll-off in phosphorescent organic light-emitting diodes** — Sebastian Wehrmeister[1], •Tobias D. Schmidt[1], Lars Jäger[1], Thomas Wehlus[2], Andreas F. Rausch[2], Thilo C. G. Reusch[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86153 Augsburg — [2]OSRAM OLED GmbH, 93049 Regensburg

We present a method for a comprehensive analysis of the efficiency roll-off with current density in phosphorescent organic light-emitting diodes (OLEDs). By combining electrical and optical excitation in time-resolved spectroscopic experiments we are able to measure the excited states lifetime for different driving conditions. It is thus possible to correlate changes of the triplet lifetime with a decrease of the radiative quantum efficiency of the emitting system due to exciton quenching processes. As compared to the conventional analysis of the measured external quantum efficiency (EQE) in dependence of the applied current density, the lifetime analysis is not affected by changes of the charge carrier balance with current, which can have a significant impact on the interpretation of the results. With this method we show that triplet-polaron quenching is the dominating quenching mechanism for the red phosphorescent emitter $\mathrm{Ir(MDQ)_2(acac)}$ doped into an $\alpha$-NPD matrix up to current densities of $100\,\mathrm{mA/cm^2}$.

CPP 76.6 Fri 11:15 C 130

**Influence of Molecular Orientation on the Coupling of Excitons to Surface Plasmons in Semitransparent Inverted Organic Solar Cells** — •Mark Gruber, Michael Mayr, Björn Gallheber, and Wolfgang Brütting — Institute for Physics, University of Augsburg, Germany

To prove the principle of coupling between surface plasmons (SPs) and excitons, we investigated semi-transparent organic solar cells, in which SPs are excited at interfaces of thin metal films and a dielectric medium by using a Kretschmann configuration setup. Therefore it is essential, that the dielectric medium has a smaller refractive index than glass, e.g. LiF or air.
To compare the SP coupling to different orientations of the transition dipole moment, two donor materials were used, diindenoperylene (DIP) and dibenzo-tetraphenyl-periflanthen (DBP). Both molecules have the transition dipole moment along the long axis. While DIP crystallizes with nearly upright standing molecules on the underlying PCBM film, DBP grows amorphous with predominantly lying molecules.[1,2] To locate the angular position of the SP resonance the reflectance of the OPVC is measured angle dependent. A simultaneously measured photo current reveals the impact of SPs in these OPVCs. The use of different donors shows, that coupling from SPs to excitons only leads to a positive effect for upright-standing transition dipole moment orientation.

[1] Wagner et al., Adv. Func. Mater. **20**, 4295, 2010.
[2] Grob et al., Appl. Phys. Lett. **104**, 213304, 2014.

**Invited Talk** CPP 76.7 Fri 11:30 C 130

**Excitonic phenomena in molecular semiconductors** — •Jens Pflaum — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ZAE Bayern, 97074 Würzburg

Excitons constitute the primary electron-hole excitation in organic solid states and offer a broad range of photo-physical phenomena. In this talk we will address two key aspects of excitonic states in molecular semiconductors: i) their sensitivity to structural ordering on various length scales and ii) their implementation as recombination sites yielding access to microscopic current characteristics.

In case of i), we will discuss the impact of molecular packing on the exciton motion [1] and how long-range exciton diffusion enables access to boundary-induced trap states that might lead to suppression of otherwise prominent singlet exciton decay channels [2]. Regarding ii), the non-invasive optical read-out of molecular recombination dynamics will be demonstrated to provide information on the local current density [3]. As a consequence, by utilizing the triplet emission of suited molecules this approach paves the way towards electrically driven single photon sources operating at room temperature [4]. Financial support within the DFG research programme SPP1355 and FOR1809 is acknowledged.

[1] A. K. Topczak, et al., Phys. Rev. B 89, 201203(R) (2014).
[2] B. Gieseking, et al., Phys. Rev. B 90, 205305 (2014).
[3] B. Stender, et al., Adv. Mater. 25, 2943 (2013).
[4] M. Nothaft, et al., Nature Comm. 3, 628 (2012).

## CPP 77: Special Session in Honor of the 75th Birthday of Siegfried Hess: Non-equilibrium dynamics of anisotropic fluids (Joint session DY, CPP)

Time: Friday 9:30–11:30 Location: BH-N 243

**Invited Talk** CPP 77.1 Fri 9:30 BH-N 243

**The "shear-gradient concentration coupling instability": non-uniform flow of sheared hard-sphere glasses.** — •Jan K.G. Dhont — Forschungszentrum Juelich, Germany

There are several types of shear-induced instabilities in soft-matter systems, like vorticity- and gradient-banding. The microscopic origin of these two instabilities is by now well understood. There is, however, an instability that can be referred to as *the Shear-gradient Concentration Coupling instability* (the SCC-instability) that has been largely ignored since its phenomenological description a few decades ago. This instability is due to a postulated shear-gradient induced mass flux together with a strong coupling of the stress to concentration. The origin of the shear-induced mass flux resulting from direct interactions is so far not understood, and explicit expressions for the corresponding transport coefficient have therefore not been derived. In this presentation, the origin of this mass flux is discussed, an explicit expression for the transport coefficient is presented, and numerical results are discussed for the stationary non-uniform flow profiles and concentration profiles of an initially SCC-unstable system, which will be compared to experiments on hard-sphere glasses.

**Invited Talk** CPP 77.2 Fri 10:00 BH-N 243

**Active anisotropic fluids** — •Sriram Ramaswamy — TIFR Centre for Interdisciplinary Sciences, Tata Institute of Fundamental Research, Hyderabad 500 075 India

The study of nonequilibrium phenomena in anisotropic fluids has taken interesting new directions recently thanks to the growing interest in the collective self-propulsion. My talk will summarise new developments from our group's work on fluids of self-driven orientable particles, in vibrated granular monolayers and active colloids.

**Invited Talk** CPP 77.3 Fri 10:30 BH-N 243

**Flow properties of anisotropic fluids** — •Sebastian Heidenreich[1], Sabine H. L. Klapp[2], and Markus Bär[1] — [1]Physikalisch Technische Bundesanstalt, Berlin, Germany — [2]Technische Universität Berlin, Berlin, Germany

From liquid crystal polymers to suspensions of bacteria anisotropic fluids are ubiquitous in nature and technology. The flow exhibits intriguing phenomena like flow alignment, shear banding, tumbling, shear thickening/thinning, large-scale correlation and mesoscale turbulence. The emergence of such fascinating aspects is often related to the anisotropy and to the out-of equilibrium character of the considered system. In the first part of our resentation we review selected flow phenomena of passive fluids with anisotropy. We discuss the role of the order parameter like the alignment tensor for the description of the flow properties. In particular, we introduce the relaxation equation for the alignment tensor coupled to the hydrodynamic flow and discuss the orientational dynamics in the shear flow. In the second part of the talk we focus on active fluids like dense bacterial suspensions and we introduce the governing hydrodynamic equations for self-sustained individuals that are swimming in a Newtonian fluid. We discuss the relationship to the passive counterpart and finally present recent work on mesoscale bacterial turbulence.

**Invited Talk** CPP 77.4 Fri 11:00 BH-N 243
**Concluding Remarks** — •Siegfried Hess — Institut für Theoretische Physik, Technische Universität Berlin, Germany

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## CPP 78: Glasses and Glass Transition (joint session CPP, DF, DY)

Time: Friday 9:30–11:15 Location: C 243

CPP 78.1 Fri 9:30 C 243
**Stable glasses from strong liquids** — •Yeong Zen Chua[1], Mathias Ahrenberg[1], Michael Tylinski[2], Mark D. Ediger[2], and Christoph Schick[1] — [1]Institute of Physics, University of Rostock, Wismarsche Str. 43-45, 18051 Rostock, Germany — [2]Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53706 USA

To date, only several materials have been observed to form ultra-stable glasses by vapor deposition. Some authors have suggested that fragility might be a controlling factor in the ability to form stable glasses by vapor deposition, with highly stable glasses only being possible for highly fragile liquids. Glasses of ethylcyclohexane, fragility index 56.5, and 1-pentene, a very small molecule, produced by physical vapor deposition have been characterized by in situ AC chip nanocalorimetry. Since the fragility index of 1-pentene was not available, it was determined as 52 from the calorimetric glass transition temperatures measured in the frequency range from 0.2 Hz to 4 kHz. Ethylcyclohexane and 1-pentene are both strong glass formers, for which possibility of stable glass formation has been questioned. On the contrary, we observed formation of highly stable glasses of ethylcyclohexane and 1-pentene. The results on ethylcyclohexane and 1-pentene will be presented and compared with literature data of other known glass formers.

CPP 78.2 Fri 9:45 C 243
**Broadband dielectric spectroscopy of ionic liquids** — •Pit Sippel[1], Michael Aumüller[1], Stephan Krohns[1,2], Peter Lunkenheimer[1], and Alois Loidl[1,2] — [1]Experimental Physics V, University of Augsburg, Germany — [2]Institute for Materials Resource Management, University of Augsburg, Germany

Due to their high potential for applications, e.g., in energy-storage devices such as supercapacitors or batteries, during recent years ionic liquids have come into the focus of research [1]. Ionic liquids are composed of organic cations and weakly coordinating anions. An essential method for the study of ionic transport is dielectric spectroscopy. Our results on a large variety of ionic liquids cover a broad frequency and temperature range. This allows obtaining valuable information on phenomena like dc charge transport, the glass transition, electrode polarization, and relaxation. We analyze the dielectric spectra using an equivalent-circuit approach [2]. Amongst others, this enables the deduction of the relaxation times of the involved dynamic processes. We conclude that the main reorientational relaxation process of these ionic liquids, the $\alpha$ relaxation, is closely linked to the dc-conductivity. This provides insight into the underlying conductivity mechanisms and, thus, the mobility of the ionic charge carriers. Moreover, a number of secondary relaxation processes is found, including hints at the presence of a Johari-Goldstein relaxation process [3].
[1] M. Armand *et al.*, Nat. Mat. **8**, 621 (2009). [2] S. Emmert *et al.*, Eur. Phy. J. B **83**, 157 (2011). [3] G.P. Johari and M. Goldstein, J. Chem. Phys. **53**, 2372 (1970).

CPP 78.3 Fri 10:00 C 243
**Dielectric spectroscopy on glycerol and water confined in metal-organic frameworks** — •Jonas Fischer[1], Pit Sippel[1], Peter Lunkenheimer[1], Dmytro Denysenko[2], Dirk Volkmer[2], and Alois Loidl[1] — [1]Experimental Physics V, University of Augsburg, Germany — [2]Chair of Solid State and Material Chemistry, University of Augsburg, Germany

Approaching the glass transition, the slowing down of molecular dynamics generally proceeds much stronger than expected for thermally activated motions. This can be ascribed to a temperature-dependent activation energy arising from the cooperative motion of increasing numbers of molecules at low temperatures [1]. The number of correlated molecules can be controlled by confining the glass-forming liquid in small pores. Previously, glass formers have been confined in porous glasses, zeolites and other silicates [2]. Recently, metal-organic frameworks (MOFs) have become available. This class of porous coordination polymers consists of metal-containing units and organic linkers. MOFs are tunable in many regards [3], thus allowing confinement in pores of different inner surfaces and varying sizes. Here, we present broadband dielectric spectroscopy data of glycerol and water confined in different MOFs, of the MFU-type [4]. It is shown that MOFs are well-suited for the measurement of confined liquids.
[1] T. Bauer *et al.*, Phys. Rev. Lett. **111**, 225702 (2013).
[2] A. Huwe *et al.*, Phys. Rev. Lett. **82**, 2338-2341 (1999).
[3] H. Furukawa *et al.*, Science **341**, 1230444 (2013).
[4] D. Denysenko *et al.*, Chem Commun. **48**, 1236 (2012).

CPP 78.4 Fri 10:15 C 243
**Dynamics of the glass transition in confined glycerol under hard and soft confinement, investigated by $^2$H NMR** — •Michael Lannert, Matthias Sattig, Thomas Blochowicz, and Michael Vogel — Hochschulstraße 6-8, 64289 Darmstadt, Germany

$^2$H NMR allows us to access correlation times of molecular rotational dynamics, ranging from $\tau$=$10^{-12}$s to $\tau$=$10^{-1}$s, by using longitudinal relaxation, solid echo, and stimulated echo sequences. Findings for confined glycerol, which is subjected to spherical soft confinement (using AOT/toluene micro-emulsions) and cylindrical hard confinement (using microporous silica, namely MCM-41) are compared, and a shift in correlation times to shorter times is observed for the hard confinement, but not for the soft confinement. Various diameters (2nm to 9nm) were used in order to gain a comprehensive understanding of the finite size effect. Investigation of the dynamics of the glycerol in the supercooled regime proved to be a challenging enterprise in soft confinement, because of the onset of rotational diffusion of the whole microemulsion droplet, which exceeds the contribution of molecular rotational dynamics. Therefore droplet size-dependence and viscosity-dependence of the dynamics where investigated additionally, in order to evaluate the impact of these results.

CPP 78.5 Fri 10:30 C 243
**Structure and Dynamics of Asymmetric Poly(styrene-*b*-1,4-isoprene) Diblock Copolymer under 1D and 2D Nanoconfinement** — •Wycliffe K. Kipnusu[1], Mahdy M. Elmahdy[1], Emmanuel U. Mapesa[1], Jiangi Zhang[2], Detlef-M. Smilgies[3], Christine M. Papadakis[4], and Friedrich Kremer[1] — [1]Institute of Experimental physics I, Linnstr.5, 04103, Leipzig — [2]National Center for Nanoscience and Technology (NCNST), No.11 ZhongGuanCun BeiYiTiao, 100190 Beijing, P.R. China. — [3]Cornell High Energy Synchrotron Source (CHESS), Wilson Laboratory, Cornell University, Ithaca, NY 14853, USA — [4]Technische Universität Müunchen, Physik-Department, Physik weicher Materie, James-Franck-Straße 1, 85748 Garching, Germany.

The impact of 1-and 2-dimensional (2D) confinement on the structure and dynamics of poly(styrene-b-1,4–isoprene) P(S-b-I) diblock copolymer is investigated by a combination of Grazing–Incidence Small–Angle X–ray Scattering (GISAXS), Atomic Force Microscopy (AFM) and Broadband Dielectric Spectroscopy (BDS). 1D confinement is achieved by spin coating the P(S-b-I) to form nanometric thin films on silicon substrates, while in the 2D confinement, the copolymer is infiltrated into cylindrical anodized aluminum oxide (AAO) nanopores. GISAXS and AFM reveal hexagonally packed cylinders of PS in a PI matrix.The dynamic glass transition of the styrene and isoprene blocks is independent of the dimensionality and the finite sizes (down to 18 nm) of confinement but the normal mode is influenced by both factors with 2D geometrical constraints exerting greater impact.

CPP 78.6 Fri 10:45 C 243

**High frequency laser heated AC-chip calorimeter for dynamic glass transition investigation in room temperature ionic liquids** — •Evgeni Shoifet[1,2,3,4], Heiko Huth[1], Sergey Verevkin[2,4], Christoph Schick[1,4], and Egon Hassel[3] — [1]Institute of Physics, University of Rostock, 18057 Rostock, Germany — [2]Institute of Physical Chemistry, University of Rostock, 18059 Rostock, Germany — [3]Department of Technical Thermodynamics, Faculty of Mechanical Engineering and Marine Technology, Rostock, 18051 Rostock, Germany — [4]Faculty of Interdisciplinary Research, Department ”Life, Light and Matter”, University of Rostock, Germany

Many ionic liquids are good glass formers. Nevertheless, for the relaxation behavior only a few studies of the dynamic glass transition in ionic liquids are available so far. Particularly the frequency dependence of the dynamic glass transition ($\alpha$-relaxation) is not known for most ionic liquids. The standard technique for such studies - dielectric spectroscopy - is not easily applicable to ionic liquids because of the high electrical conductivity. In addition, dielectric spectroscopy is equally sensitive to the segmental relaxation ($\alpha$-relaxation) and secondary relaxation but calorimetry is sensitive solely to segmental relaxation.

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. Particularly the influence of alkyl chain length on the $\alpha$-relaxation in the frequency range from 1 mHz to 0.1 MHz [Shoifet. E. et. al. (2013)].

CPP 78.7 Fri 11:00 C 243

**Dynamic glass transition measurements on nm-thin films of Indomethacin using AC chip-nanocalorimetry** — •Mathias Ahrenberg, Christoph Schick, and Gunnar Schulz — Institut für Physik, Universität Rostock

We are using AC chip nano-calorimetry for the in-situ investigation of the dynamic glass transition of vapor-deposited thin films of toluene and indomethacin of thicknesses between several hundred nm down to ten nm. With these experiments on low molecular mass substances we complement our data on similar thin polymer films. Firstly, the deposition-related thermodynamic state (stable glass) of each film is erased by transforming them into ordinary glasses. Secondly, upon reheating the thin ordinary glass films a direct comparison of the subsequently measured frequency-dependent dynamic glass transition temperatures becomes possible. The frequency of temperature modulation can be varied from 1 Hz up to about 1000 Hz. Film thicknesses for indomethacin are measured ex-situ with an atomic force microscope directly on the membrane of the chip-sensors. Similar to the thin polymer films no thickness dependence of the dynamic glass transition temperature (main relaxation) is seen. The results are in agreement with the explanation given by Cangialosi et al.

## CPP 79: Microswimmers, Active Liquids II (joint session CPP, BP, DY)

Time: Friday 9:30–11:30 Location: C 264

**Invited Talk** CPP 79.1 Fri 9:30 C 264

**From chemical nanomotors to biological microswimmers** — •Peer Fischer — Max-Planck-Institut für Intelligente Systeme, Heisenbergstr. 3, 70569 Stuttgart — Institut für Physikalische Chemie, Universität Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart

Building, powering, and operating structures that can navigate complex fluidic environments at the sub-mm scale is challenging. Moving through fluid environments at the scale of micro-organisms for instance presents a different set of challenges compared to those encountered by macroscopic swimmers. Artificial means of realizing motion in microparticles often makes use of local gradients that are established across the colloid, resulting in slip velocities at the particle surface, which in turn drives the motion. In its simplest form this can be realized with Janus-like colloids. I describe what, to the best of my knowledge, are the smallest synthetic chemical nanomotors that have been made and show that their active motion can be tracked with light scattering. Moving from enhanced diffusion to propulsion, I present recent results where colloidal nanopropellers can be moved in water by external magnetic fields similar to a bacterial flagellum and show how the motion of these structures can benefit from the complex rheology in biological media. Although strong Brownian forces dominate in water we achieve controlled propulsion in biological gels, which paves the way for applications inside biological media and the extracellular matrix. Finally, I present an example of a microscallop that does not move in water, but that swims in non-Newtonian liquids.

CPP 79.2 Fri 10:00 C 264

**Optothermal Manipulation of Plasmonic Nanoparticles in Viscous Solvents** — •Felix Winterer[1,2], Christoph Maier[1,2], Theobald Lohmüller[1,2], and Jochen Feldmann[1,2] — [1]Photonics and Optoelectronics Group, Ludwig-Maximilians-Universität München, Munich, Germany — [2]Nanosystems Initiative Munich (NIM), Munich, Germany

We present an all-optical approach to move and manipulate single plasmonic nanoparticles with high accuracy in viscous solvents.

Gold nanoparticles are subject to optical forces and heat generation upon irradiation with a focussed laser beam. Tuning the laser wavelength with respect to the plasmon resonance frequency allows for switching between repulsive and attractive optical forces, which renders it possible to trap or push individual nanoparticles in two and three dimensions. At the same time, laser light can induce heat in the surrounding medium.

We explore how both effects can be employed to control nanoparticle movement by a combination of thermal gradients and optical forces and discuss further applications of this approach for nanolithography and nanoscale physics.

CPP 79.3 Fri 10:15 C 264

**Dynamics of a carpet of self-propelled surfactant particles covering a liquid film** — Andrey Pototsky[1], •Uwe Thiele[2], and Holger Stark[3] — [1]Department of Mathematics, Swinburne University of Technology, Hawthorn, Victoria, 3122, Australia — [2]Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [3]Institut für Theoretische Physik, Technische Universität Berlin, 10623, Berlin, Germany

We consider a carpet of self-propelled surface-active particles that move along the liquid-gas interface of a liquid film on a solid substrate and whose swimming direction changes in time due to rotational diffusion. We study the intricate influence of these self-propelled insoluble surfactants on the stability of the film surface and show that depending on the strength of in-surface rotational diffusion and the absolute value of the in-surface velocity several instability modes can occur [1]. In particular, the rotational diffusion can have a stabilizing or destabilizing influence and may even suppress the instability entirely. In the limit of purely upwards swimming we recover the destabilisation described in the literature [2]. The results of the linear analysis are confirmed by fully nonlinear simulations of the complete continuum model and as well through a hybrid discrete self-propelled surfactant particles - continuous film model. [1] A. Pototsky, U. Thiele and H. Stark, Phys. Rev. E **90**, 030401(R) (2014). [2] S. Alonso and A.S. Mikhailov, Phys. Rev. E **79**, 061906 (2009).

CPP 79.4 Fri 10:30 C 264

**Tangled Flagella: Importance in Bacterial Propulsion** — •Tapan Chandra Adhyapak and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, D - 10623 Berlin

It has been well established that hydrodynamic interactions between flagella of peritrichous bacteria such as E. coli, leads to synchronization of rotation and bundling of those flagella [1,2]. Flagella are rotated at their bases by rotary motors embedded in the cell body. In response, the cell body has to rotate in the opposite sense such that total torque acting on the bacterium is zero. Often, such cell rotation causes flagella to tangle before they are synchronized completely. We show that tangling has a profound effect on the overall synchronization and bundling dynamics. In particular, we observe abrupt synchronization and bundling on time scales much shorter than those required when the cell movement is switched off to avoid entanglement. Although hydrodynamic interactions still play an important role, through a comparative investigation we conclude that flagellar entanglement generated by cell rotation predominantly affects the total time to synchronize

and bundle. Cell movement modifies stationary bundling states too. Specifically, the length over which a bundle is closely pact varies over time, having an oscillatory behavior whose amplitude decreases with increasing number of flagella. At the end we discuss how strongly all these findings affect the overall propulsion of the bacterium.
[1] M. Reichert and H. Stark, Eur. Phys. J. E **17**, 493 (2005).
[2] S.Y. Reigh, R.G. Winkler, and G. Gompper, Soft Matter **8**, 4363 (2012).

CPP 79.5 Fri 10:45 C 264

**Reorientation of passive Janus type swimmer in an external temperature profile** — •Andreas Bregulla and Frank Cichos — University of Leipzig, department for experimental physics, leipzig, germany

Swimming on the micrometer length scale is dominated by omnipresent Brownian fluctuations and overwhelming viscous forces. Self-phoretic swimmers are an example how to overcome those limitations. Most of those particles are driven by phoretic surface flows generated by surface gradients. In the last decade many different phoretic swimming mechanisms have been proposed. When such self-propelled objects are starting to interact at higher densities, coherent collective motions are observed in which the swimmers align and form flocks, swarms or other complicated patterns. About the origin and details of these complex interactions only little is known. The lack of understanding is mostly due to the lack of control of such particles. Here we want to present a method which extends the existing photon nudging algorithm to gather and collect a specific number of particles and study their interactions. The interactions themselves can be mediated through many different aspects like charges, flow fields or through external profiles created by each active swimmer. The last mentioned interaction will be discussed in detail. An immobile gold colloid acts as an external heat source and mimics the temperature profile that an active swimmer would create in its surrounding. The motion of a passive Janus particle in this temperature field is investigated and the relative motion and alignment with respect to the heat source is quantified.

CPP 79.6 Fri 11:00 C 264

**Thermophoretic Trapping of Single and Multiple Nano-Objects by Actively Controlled Temperature Fields** — •Marco Braun and Frank Cichos — Molecular Nanophotonics, Fakultät für Physik und Geowissenschaften, Universität Leipzig, Deutschland

The understanding of nano-scale soft-matter science benefited enormously from the ability to study single molecules, such as DNA or proteins. In solution Brownian motion lets a molecule disappear quickly from the observation volume, which is why it is typically immobilized in a polymer matrix or by chemical interactions, generally accepted due to a lack of alternatives. However, this strongly changes the local physical and chemical properties. Here, we present an all-optical technique to trap single nano-objects in solution which exploits highly localized temperature fields. The so-called thermophoretic trap exploits thermophoretic interactions of a particle with a temperature gradient, which e.g. locally distorts the screening of the surface charges and by that induces a drift of the particle. 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 particle 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. The real-time control of the laser beam thereby allows for arbitrary effective trapping potentials for single and multiple particles.

CPP 79.7 Fri 11:15 C 264

**Low-tech, high-throughput tracking of bacteria in 3D** — •Katja Taute, Sander Tans, and Tom Shimizu — FOM Institute AMOLF, Science Park 102, Amsterdam 1098XG, The Netherlands

Many bacteria swim in liquids and execute complex motility patterns. The increasingly recognized diversity of motility strategies has sparked a growing interest in their characterization via 3D tracking. The only 3D tracking techniques thus far to have passed the benchmark of resolving the model bacterium E. coli's run-tumble motility suffer from being limited to single individuals [1]; and/or are technically challenging and require specialized experimental setups [1,2,3].

Here we present a broadly applicable high-throughput 3D bacterial tracking technique which requires only a standard biological phase contrast microscope. We exploit the relationship between an object's distance to the focal plane (z) and the observed intensity pattern, and assign z positions by maximizing image cross-correlations to a reference stack. We achieve micron-scale resolution in z, <0.5 $\mu$m resolution in x and y, a range of ~350x300x200 $\mu$m (x,y,z), a throughput of tens of bacteria, and a temporal resolution that is only limited by the detector readout rate. We demonstrate the application of this technique to a range of bacterial species, verify that we recover previously observed motility patterns, and reveal that bacterial individuality, rather than stochasticity, underlies the broad population distribution observed for a key motility parameter of V. alginolyticus.

[1] Berg & Brown, Nature 239:500, 1972. [2] Vater et al., PLoS ONE 9:e87765, 2014. [3] Molaei et al., PRL 113:068103, 2014.

## CPP 80: Transport: Molecular Electronics (joint session with TT, CPP, HL, MA, O)

Time: Friday 9:30–12:15 Location: H 0110

CPP 80.1 Fri 9:30 H 0110

**Phononic and thermoelectric properties of $\pi$-stacked molecular junctions** — •Thomas Hellmuth[1,3], Marius Bürkle[2], and Fabian Pauly[1] — [1]Theorie der Nanostrukturen, Universität Konstanz, 78457 Konstanz, Germany — [2]Nanosystem Research Institute, National Institute of Advanced Industrial Science and Technology, Japan — [3]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76131 Karlsruhe,Germany

We present our newly developed approach to compute phonon thermal transport through nanosystems from first principles using density functional theory combined with non-equilibrium Green's function techniques. Combining both electron and phonon transport, we analyze the heat transport and thermoelectric properties of $\pi$-stacked paracyclophane molecules contacted to gold electrodes [1]. We show that, depending on temperature, the phononic contribution to the heat conductance is a factor of about 5 larger than the electronic one. By calculating the thermoelectric coefficients in linear response, we estimate the figure of merit $ZT$ of the single-molecule junctions for different molecular lengths and substituents.

[1] M. Bürkle, T. J. Hellmuth, F. Pauly, Y. Asai, submitted.

CPP 80.2 Fri 9:45 H 0110

**Conductance and thermopower of $C_{82}$ and endohedral metallofullerene molecular junctions with Au electrodes** — •Marius Buerkle[1], See Kei Lee[2], Ryo Yamada[2], Hirokazu Tada[2], and Yoshihiro Asai[1] — [1]AIST, NRI, Tsukuba, Japan — [2]Graduate School of Engineering Science, Osaka University, Japan

By combining STM based conductance and thermopower measurements with first-principle transport calculations we investigate the thermoelectric properties of single $C_{82}$ molecules, and its endohedral metallofullerene (EMF) derivatives Gd@$C_{82}$ and Ce@$C_{82}$ bridging Au electrodes. All three molecular junctions show a comparable conductance of around 0.2 G0 and a negative thermopower indicating electron-like transport through the lowest unoccupied molecular orbital (LUMO). However, for the EMF junctions a much larger thermopower is observed which we can relate to changes in the electronic structure induced by the lanthanide atoms.

CPP 80.3 Fri 10:00 H 0110

**A scaling relation in the vibronic contribution to the current noise** — •Yoshihiro Asai — AIST, Tsukuba, Japan

The electron-phonon coupling effect on the electric current noise is studied based on the fully self-consistent theory of electron and phonon currents (SCEPC) given in terms of the Keldysh Greens function method [1], which has been successful in describing the local heating phenomena [2] and the temperature dependence of the electric conductance [3,4]. Based on the theoretical result on the noise accompanying the vibronic current, we will discuss a scaling relation between the two quantities derived from the current noise and the electric conductance at finite bias voltage. We found that the scaling relation holds when the dynamics of the electron satisfies a specific condition. We will describe these in the talk.

[1] Y. Asai, Phys. Rev. B 78, 045434-1-24 (2008).
[2] Y. Asai, Phys. Rev. B, 84, 085436-1-7 (2011).
[3] S.-K. Lee, R. Yamada, S.Tanaka, G.-S. Chang, Y. Asai, and H. Tada, ACS Nano, 6, 5078-5082 (2012).
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CPP 80.4 Fri 10:15 H 0110

**Thermo-voltage of nano-thermocouples** — •Ayelet Ofarim, Bastian Kopp, Johannes Boneberg, Paul Leiderer, and Elke Scheer — University of Konstanz, Department of Physics, Konstanz, Germany

As the down-scaling of electronic components continues, engineering the devices has become a challenge, in particular in view of energy and heat management. Study of thermoelectric effects in nanostructures gives important additional information about charge transport, also regarding possible life-time limiting phenomena and applications for the conversion of light energy via heat into electrical energy. The scope of this presentation is to gain deep insight into the charge transport mechanism, by studying thermo-voltage effects of metallic atomic-sized contacts [1]. We present the concept for determination of the thermo-voltage of nano-thermocouples, using a novel mechanically-controlled break junction (MCBJ) mechanism. A technique to create and detect a temperature gradient, using laser irradiation, is also presented.

[1] B. Kopp, Z. Yi, D. Benner, F. Q. Xie, C. Obermair, T. Schimmel, J. Bonenberg, P. Leiderer and E. Scheer,
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CPP 80.5 Fri 10:30 H 0110

**Quantum interference in thermoelectric molecular junctions: A toy model perspective** — •Daijiro Nozaki[1], Stas. M. Avdoshenko[2], Haldun Sevinçli[3], and Gianaurelio Cuniberti[1,4,5] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [2]Department of Chemistry and Institute for Computational Engineering and Sciences, University of Texas at Austin, USA — [3]Department of Materials Science and Engineering, Izmir Institute of Technology, Turkey — [4]Dresden Center for Computational Materials Science (DCCMS), TU Dresden, Germany — [5]Center for Advancing Electronics Dresden (cfAED), TU Dresden, Germany

In order to reveal the relationship between the line shape of the transmission spectra affected by quantum interference and the electronic structures, we consider a homogeneous toy model where all on-site energies are identical and model four types of molecular junctions due to their topological connectivities. We systematically analyze their transmission spectra, density of states, and thermoelectric properties. Even without the degree of freedom for on-site energies an asymmetric Fano peak could be realized in the homogeneous systems with the cyclic configuration. We also calculate the thermoelectric properties of the model systems with and without fluctuation of on-site energies. Even under the fluctuation of the on-site energies, the finite thermoelectrics are preserved for the Fano resonance, thus cyclic configuration is promising for thermoelectric applications.

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J. Appl. Phys. 117, 074308 (2014).

CPP 80.6 Fri 10:45 H 0110

**Effect of nonadiabatic electronic-vibrational interactions on the transport properties of single-molecule junctions** — •André Erpenbeck[1], Rainer Härtle[2], and Michael Thoss[1] — [1]Institut für Theoretische Physik und Interdisziplinäres Zentrum für Molekulare Materialien (ICMM), Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany — [2]nstitut für theoretische Physik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany

The interaction between electronic and vibrational degrees of freedom in single-molecule junctions may result from the dependence of the electronic energies or the electronic states of the molecular bridge on the nuclear displacement. The latter mechanism leads to a direct coupling between different electronic states and is referred to as nonadiabatic electronic-vibrational coupling. Employing nonequilibrium Green's functions in combination with the self-consistent Born approximation, we study the influence of nonadiabatic electronic-vibrational coupling in model molecular junctions. Thereby we distinguish between systems with well separated and quasi-degenerate electronic levels. Our results show that the nonadiabatic electronic-vibrational interaction can have a significant influence on the transport properties [1]. The underlying mechanisms are analyzed with respect to the different signatures of nonadiabatic and adiabatic electronic-vibrational coupling, the relevant transport channels, negative differential resistance and quantum interference effects.

[1] A. Erpenbeck et. al., arXiv:1411.5844 (2014)

**15 min. break.**

CPP 80.7 Fri 11:15 H 0110

**Significant role of end groups in electrical transport through molecules** — •Karthiga Kanthasamy[1], Markus Ring[2], Fabian Pauly[2], Christoph Tegenkamp[1], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik, Leibniz Universität, Hannover, Germany — [2]Fachbereich Physik, Universität Konstanz, Germany

Mechanically controllable break junction (MCBJ) technique is used to investigate the electronic properties of ferrocene and phenyl based molecules with different end groups. Stepwise changes in conductance are observed below 1Go after insertion of the molecules. The junctions are opened in vacuum and IV curves are measured for various distances between the electrodes. Detailed analysis of IV curves shows characteristic peaks in the first-order derivative for ferrocene dithiol (FDT) molecules, which are absent in ferrocene diamine (FDA) and biphenyl dithiol (BPDT). For FDT, in the range of 0.56Go to 0.09Go, there are two symmetric peaks, whose energy difference increases from 60 meV to 160 meV with increasing contact distance. Above 0.56Go or below 0.01Go, symmetric peaks are absent. The FDT molecules show typically a one order of magnitude higher conductance than FDA and BPDT. The IV graph for FDT is linear, i.e., it has metallic characteristics, while FDA and BPDT are dominated by tunneling. Theoretical calculations for the molecules in different configurations between the gold electrodes are performed based on density functional theory and the non-equilibrium Green's function formalism. Both elastic transport properties and inelastic electron tunneling spectra are studied to explain the experimental observations.

CPP 80.8 Fri 11:30 H 0110

**Photoinduced transient current through a molecular junction: Effects of lead excitation** — •Yaroslav Zelinskyy[1,2], Yoram Selzer[3], and Volkhard May[1] — [1]Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, D-12489 Berlin, Germany — [2]Bogolubov Institute for Theoretical Physics, National Academy of Science of Ukraine, 14-b Metrologichna str., UA-03683, Kiev, Ukraine — [3]School of Chemistry, Tel Aviv University, Ramat Aviv, 69978 Tel Aviv, Israel

Laser pulse induced transient currents through a molecular junction are studied in the framework of a density matrix theory. By focusing on the sequential transport regime two types of lead excitation are considered. Firstly, effects of collective plasmon excitations of the leads and their resonant coupling to molecular excitations are investigated. If such a resonant coupling cannot be realized a second excitation regime would be of interest. Now, the nonequilibrium dynamics of individual lead electrons affect the transient current formation. While a resonant coupling to lead plasmon excitations induces a remarkable current enhancement nonequilibrium electron distributions in the leads determine the transient current mainly by their thermalization process. The theoretical framework described above is used to analyze time-resolved conductance measurements of molecular junctions based on Ferrocene molecules.

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[3] Y. Zelinskyy, Y. Selzer and V. May, Phys. Rev. B (submitted)).

CPP 80.9 Fri 11:45 H 0110

***Ab-initio* model of extended CNT-metal contact** — Artem Fediai[1,2,3], •Dmitry Ryndyk[1,2,3], and Gianaurelio Cuniberti[1,2,3] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [3]Dresden Center for Computational Materials Science (DCCMS), TU Dresden, 01062 Dresden, Germany

Relevant CNT-metal contacts belong to so-called extended type. Current flows from electrodes into CNT in a distributed manner, and contact resistance depends on the contact length. In such circumstances the standard *ab-initio* based transport techniques to calculate electron transport should be modified.

We have developed a special method which allows calculation of transport in the systems with metal-CNT contacts at *ab-initio* level. It takes into account both internal and external parts of the CNT-metal contact and requires simulation of the one principal and two auxiliary atomistic systems. Results of *ab-initio* calculations are then subjected to special treatment and being used in Green function formalism afterwards.

This method was applied to Al-CNT and Pd-CNT extended contacts. Results agree perfectly with existing experimental data being indeed obtained at a purely *ab-initio* level.

CPP 80.10 Fri 12:00 H 0110

**Hierarchical Quantum Master Equation Approach to Vibrationally Coupled Electron Transport in Single-Molecule Junctions** — •Christian Schinabeck[1], Rainer Härtle[2], and Michael Thoss[1] — [1]Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany — [2]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany

We investigate vibrationally coupled transport in single-molecule junctions using the hierarchical quantum master equation (HQME) approach [1-3]. This method allows a systematic convergence of the reduced dynamics of open quantum systems beyond the traditional Markovian rate equations. Within the HQME framework, two different approaches are presented and compared, which describe the vibrational degrees of freedom as part of the system or the bath, respectively. The methodology is applied to a model molecular junction consisting of a molecular level coupled to fermionic leads as well as a vibrational mode. For this system, the accurate results of the hierarchical quantum master equation approach are compared with Markovian rate equation as well as fourth-order time-nonlocal master equation calculations in different parameter regimes. The convergence properties of the two HQME approaches are analyzed in detail.

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