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

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Overview of Invited Talks and Sessions

(Lecture rooms ZEU 114, ZEU 160, ZEU 222, ZEU 250, ZEU 255, ZEU 260, HSZ 02, and SCH A251;
Poster P1A, P1C, P2-OG1, and P3)

Invited Talks

CPP 1.1	Mon	9:30–10:00	ZEU 222	**Dynamically Reconfigurable Soft Matter in External Fields: Smart Particle Gels, Shape-Changing Clusters and Self-Propelling Microbots** — •Orlin D Velev
CPP 3.1	Mon	10:15–10:45	ZEU 222	**The Versatility of Mesoscopic Solar Cells** — •Anders Hagfeldt
CPP 4.1	Mon	10:15–10:45	ZEU 114	**Membrane nanotube formation in giant vesicles** — •Rumiana Dimova
CPP 5.1	Mon	10:15–10:45	ZEU 255	**A Combined Rheological and Dielectric Analysis of Filler Networking in Elastomer Nano-Composites** — •Manfred Klüppel
CPP 8.1	Mon	15:00–15:30	ZEU 222	**Visualizing Charge Carrier Diffusion In Hybrid Halide Perovskite Thin Films** — •Achim Hartschuh, Kathrin Handloser, Irene Grill, Nicolai Hartmann, Nadja Giesbrecht, Meltem Aygüler, Mathhias Handloser, Thomas Bein, Pablo Docampo
CPP 8.2	Mon	15:30–16:00	ZEU 222	**Photon recycling in hybrid lead-halide perovskite semiconductors** — •Felix Deschler
CPP 8.5	Mon	16:45–17:15	ZEU 222	**Interface engineering: the route towards high efficiency and stable hybrid perovskite solar cells** — •Giulia Grancini
CPP 9.1	Mon	15:00–15:30	ZEU 260	**Molecular Electrical Doping of Organic Semiconductors** — •Ingo Salzmann
CPP 20.1	Tue	9:30–10:00	ZEU 222	**Investigation of hybrid organic/inorganic perovskite systems and interfaces by photoelectron spectroscopy** — •Selina Olthof
CPP 22.7	Tue	11:15–11:45	ZEU 250	**Structure/dynamics interplay in interfacial layers: how adsorption influences thermal glass transition and segmental relaxation** — •Simone Napolitano
CPP 22.10	Tue	12:15–12:45	ZEU 250	**Molecular-level framework for the dynamic mechanical response and yielding of polymer glasses** — •Alessio Zaccone, Vladimir Palyulin, Chris Ness, Robert Elder, Rico Milkus, Timothy Sirk
CPP 25.1	Tue	14:00–14:30	ZEU 222	**Ultrafast transient absorption spectroscopy of organic-inorganic hybrid perovskites on mesoporous titanium dioxide in contact with hole transport materials** — •Thomas Lenzer
CPP 31.1	Wed	9:30–10:00	ZEU 222	**Using classical polymer science tools to manipulate phase transformations, solid-state order and properties of semiconducting plastics – and beyond** — •Natalie Stingelin
CPP 35.6	Wed	11:45–12:15	ZEU 222	**Density functional theory of crystallization: from anisotropic particles to polymers** — •Hartmut Loewen
CPP 36.1	Wed	10:15–10:45	ZEU 260	**Computer simulations of colloidal systems under flow** — •Arash Nikoubashman
CPP 37.5	Wed	11:15–11:45	ZEU 255	**Nonlinear dielectric spectroscopy in supercooled liquids** — Peter Lunkenheimer, Marion Michl, Thomas Bauer, Francois Ladieu, Samuel Albert, •Alois Loidl

CPP 38.1	Wed	10:15–10:45	ZEU 250	**Light-induced degradation of methylammonium and formamidinium PbI3 perovskites** — •Norbert H. Nickel, Felix Lang, Victor V. Brus, Jörg Rappich
CPP 40.1	Wed	15:00–15:30	ZEU 222	**Architectural Engineering of Semi-Crystalline Elastomers** — •Sergei Sheiko
CPP 40.5	Wed	16:30–17:00	ZEU 222	**Chain Trajectory of Semicrystalline Polymers as Revealed by Solid-State NMR Spectroscopy** — •Toshikazu Miyoshi
CPP 40.9	Wed	17:45–18:15	ZEU 222	**The Role of Entanglement in Polymer Crystallization** — •Chuanfu Luo
CPP 41.1	Wed	15:00–15:30	ZEU 260	**The role of incoherent hopping in the photogeneration of charges in organic semiconductors** — •Anna Köhler
CPP 42.5	Wed	16:00–16:30	ZEU 114	**Aqueous Ionic Liquids and Their Influence on Peptide Conformations: Denaturation and Dehydration Mechanisms** — •Jens Smiatek
CPP 47.1	Wed	16:15–16:45	ZEU 255	**Hard science with soft spheres: learning from foams and emulsions** — •Wiebke Drenckhan-Andreatta
CPP 53.1	Thu	9:30–10:00	ZEU 222	**Interplay of Order and Disorder in Self-assembled Optical Metamaterials** — •Ullrich Steiner
CPP 55.1	Thu	10:15–10:45	ZEU 222	**Understanding charge transport in crystalline organic semiconductors** — •Simone Fratini, Sergio Ciuchi, Alessandro Troisi, Didier Mayou
CPP 55.2	Thu	10:45–11:15	ZEU 222	**Mapping of trap densities and contact resistance in organic devices and their relation to structural disorder** — •Bert Nickel, Clemens Liewald, Simone Strohmair, Eric Glowacki, Andrey Turchanin
CPP 56.1	Thu	10:15–10:45	ZEU 260	**Functional microgels: simple matter where complexity matters** — •Walter Richtering
CPP 58.4	Thu	11:00–11:30	ZEU 255	**Molecular Scale Structure of Ionic Liquid Surfaces** — •Markus Mezger
CPP 59.1	Thu	15:00–15:30	ZEU 222	**Charge transport modeling in disordered molecular semiconductors: from the molecule to the device** — Andrea Massé, Feilong Liu, Pascal Friederich, Franz Symalla, Velimir Meded, Wolfgang Wenzel, Reinder Coehoorn, •Peter A. Bobbert
CPP 59.2	Thu	15:30–16:00	ZEU 222	**Charge transport in high mobility molecular semiconductors** — •Henning Sirringhaus
CPP 60.1	Thu	15:00–15:30	ZEU 260	**Polymers in the cell nucleus** — •Maria Barbi, Antony Lesage, Jean-Marc Victor
CPP 60.6	Thu	16:45–17:15	ZEU 260	**Knots as Stable Topological Order Parameter for Semiflexible Polymers** — •Wolfhard Janke, Martin Marenz
CPP 63.1	Fri	9:30–10:00	ZEU 222	**Stimuli-Responsive and Switchable Polymer Brushes: Theoretical Concepts and Computer Simulations** — •Jens-Uwe Sommer
CPP 67.4	Fri	11:00–11:30	ZEU 222	**Protein Folding under Mechanical Load** — •Matthias Rief
CPP 67.6	Fri	12:00–12:30	ZEU 222	**All-atom simulations of folding of proteins with topologically complex native structures.** — •Pietro Faccioli, Silvio a Beccara
CPP 70.5	Fri	11:15–11:45	ZEU 255	**Charge transfer states for organic opto-electronics** — •Koen Vandewal

Tutorial Patterns in Nature und Materials

DY 1.1	Sun	16:00–16:50	HSZ 04	**The fascination of pattern formation: Basic principles, applications, future directions** — •Walter Zimmermann
DY 1.2	Sun	16:50–17:40	HSZ 04	**On growth and forms in nature** — •Chaouqi Misbah
DY 1.3	Sun	17:40–18:30	HSZ 04	**What can pattern formation theory tell us about ecosystem response to climate change?** — •Ehud Meron

Invited talks of the joint symposium SYBM

See SYBM for the full program of the symposium.

SYBM 1.1	Tue	9:30–10:00	HSZ 02	**New twists in biological photonics: circular polarisation and beyond.** — •Pete Vukusic, Luke McDonald, Ewan Finlayson

SYBM 1.2	Tue	10:00–10:30	HSZ 02	**Bio-inspired materials and structures for technology and architecture** — •Thomas Speck
SYBM 1.3	Tue	10:30–11:00	HSZ 02	**Cellulose bio-inspired hierarchical structures** — •Silvia Vignolini
SYBM 1.4	Tue	11:15–11:45	HSZ 02	**Strong Flexible Bioenabled Nanocomposites for Sustainable Sensing** — •Vladimir Tsukuruk
SYBM 1.5	Tue	11:45–12:15	HSZ 02	**3D laser nano-printing of rationally designed materials** — •Martin Wegener

Invited talks of the joint symposium SYES

See SYES for the full program of the symposium.

SYES 1.1	Fri	10:30–11:00	HSZ 02	**Going Beyond Conventional Functionals with Scaling Corrections and Pairing Fluctuations** — •Weitao Yang
SYES 1.2	Fri	11:00–11:30	HSZ 02	**Multi-reference density functional theory** — •Andreas Savin
SYES 1.3	Fri	11:30–12:00	HSZ 02	**Density functionals from machine learning** — •Kieron Burke
SYES 1.4	Fri	12:00–12:30	HSZ 02	**Taming Memory-Dependence in Time-Dependent Density Functional Theory** — •Neepa Maitra
SYES 1.5	Fri	12:30–13:00	HSZ 02	**Quantum Embedding Theories** — •Fred Manby

Sessions

CPP 1.1–1.1	Mon	9:30–10:00	ZEU 222	**Keynote Lecture I**
CPP 2.1–2.10	Mon	9:30–13:00	SCH A251	**Mechanics and Dynamics of 3D Tissues (joint focus session BP/CPP, organized by BP)**
CPP 3.1–3.9	Mon	10:15–13:00	ZEU 222	**Fundamentals of Perovskite Photovoltaics I (joint session CPP/DS/HL)**
CPP 4.1–4.9	Mon	10:15–13:00	ZEU 114	**Bioinspired Functional Materials I**
CPP 5.1–5.9	Mon	10:15–13:00	ZEU 255	**Polymer Networks and Dynamics I: Elastomers and Magnetic Materials**
CPP 6.1–6.9	Mon	10:15–13:15	ZEU 160	**Focus: Soft Particles in Flows I (joint focus session CPP/DY)**
CPP 7.1–7.8	Mon	11:00–13:00	ZEU 260	**Organic Electronics and Photovoltaics I: Light-Emitting Devices (joint session CPP/DS/HL, organized by CPP)**
CPP 8.1–8.9	Mon	15:00–18:15	ZEU 222	**Fundamentals of Perovskite Photovoltaics II (joint session CPP/DS/HL)**
CPP 9.1–9.11	Mon	15:00–18:15	ZEU 260	**Organic Electronics and Photovoltaics II: Doping (joint session CPP/DS/HL, organized by CPP)**
CPP 10.1–10.12	Mon	15:00–18:15	ZEU 114	**Bioinspired Functional Materials II**
CPP 11.1–11.12	Mon	15:00–18:15	ZEU 255	**Modelling and Simulation of Soft Matter**
CPP 12.1–12.10	Mon	15:00–18:00	ZEU 160	**Focus: Soft Particles in Flows II (joint focus session CPP/DY)**
CPP 13.1–13.30	Mon	18:30–21:00	P1A	**Poster: Fundamentals of Perovskite Photovoltaics (joint session CPP, DS, HL)**
CPP 14.1–14.8	Mon	18:30–21:00	P1C	**Poster: Bioinspired Functional Materials**
CPP 15.1–15.13	Mon	18:30–21:00	P1C	**Poster: Membranes, Biomaterials, Biopolymers**
CPP 16.1–16.6	Mon	18:30–21:00	P1C	**Poster: Modelling and Simulation of Soft Matter**
CPP 17.1–17.10	Mon	18:30–21:00	P1C	**Poster: Polymer Networks and Dynamics**
CPP 18.1–18.14	Mon	18:30–21:00	P1C	**Poster: Colloids and Complex Fluids**
CPP 19.1–19.5	Tue	9:30–12:15	HSZ 02	**Symposium on Bioinspired Functional Materials: From Nature's Nanoarchitectures to Nanofabricated Designs**
CPP 20.1–20.10	Tue	9:30–12:30	ZEU 222	**Fundamentals of Perovskite Photovoltaics III (joint session CPP/DS/HL)**
CPP 21.1–21.12	Tue	9:30–12:45	ZEU 260	**Organic Electronics and Photovoltaics III: Mobile and Trapped Charges (joint session CPP/DS/HL, organized by CPP)**
CPP 22.1–22.10	Tue	9:30–12:45	ZEU 250	**Polymer Networks and Dynamics II: Structure and Dynamics**
CPP 23.1–23.13	Tue	9:30–13:15	POT 251	**Organic Semiconductors (joint session CPP/DS/HL, organized by HL)**

CPP 24.1–24.6	Tue	11:30–13:00	ZEU 255	**Colloids and Complex Fluids I (joint session BP/CPP/DY, organized by CPP)**
CPP 25.1–25.7	Tue	14:00–16:00	ZEU 222	**Fundamentals of Perovskite Photovoltaics IV (joint session CPP/DS/HL)**
CPP 26.1–26.8	Tue	14:00–16:00	ZEU 260	**Molecular Electronics and Excited State Properties**
CPP 27.1–27.7	Tue	14:00–15:45	ZEU 114	**Photoswitchable Materials**
CPP 28.1–28.6	Tue	14:00–15:45	ZEU 160	**Focus: Soft Particles in Flows III (joint focus session CPP/DY)**
CPP 29.1–29.8	Tue	14:00–16:00	ZEU 250	**Polymer Networks and Dynamics III: Mechanical Properties**
CPP 30.1–30.12	Wed	9:30–12:45	HSZ 201	**Transport: Molecular Electronics and Photonics (jointly with CPP, HL, MA, O)**
CPP 31.1–31.1	Wed	9:30–10:00	ZEU 222	**Keynote Lecture II**
CPP 32.1–32.14	Wed	9:30–13:15	CHE 91	**Organic Thin Films I (joint session CPP/DS/HL, organized by DS)**
CPP 33.1–33.11	Wed	9:30–12:45	POT 81	**Organic Photovoltaics and Electronics I (joint session CPP/DS/HL, organized by HL)**
CPP 34.1–34.6	Wed	9:30–12:30	GER 37	**Focus: Spatio-Temporal Multiscale Optical Spectroscopy Meets Functional Materials (joint session DF/CPP/O, organized by DF)**
CPP 35.1–35.9	Wed	10:15–13:00	ZEU 222	**Focus: Polymer Crystallization - from Model Systems to New Materials I**
CPP 36.1–36.9	Wed	10:15–13:00	ZEU 260	**Colloids and Complex Fluids II (joint session BP/CPP/DY, organized by CPP)**
CPP 37.1–37.9	Wed	10:15–13:00	ZEU 255	**Fluids and Glasses I**
CPP 38.1–38.8	Wed	10:15–12:45	ZEU 250	**Fundamentals of Perovskite Photovoltaics V (joint session CPP/DS/HL)**
CPP 39.1–39.10	Wed	14:45–17:45	POT 81	**Organic Photovoltaics and Electronics II (joint session CPP/DS/HL, organized by HL)**
CPP 40.1–40.9	Wed	15:00–18:15	ZEU 222	**Focus: Polymer Crystallization - from Model Systems to New Materials II**
CPP 41.1–41.12	Wed	15:00–18:30	ZEU 260	**Organic Electronics and Photovoltaics IV: OPV (joint session CPP/DS/HL, organized by CPP)**
CPP 42.1–42.10	Wed	15:00–18:00	ZEU 114	**Charged Soft Matter, Ionic Liquids and Polyions I**
CPP 43.1–43.4	Wed	15:00–16:00	ZEU 255	**Fluids and Glasses II**
CPP 44.1–44.15	Wed	15:00–19:00	HÜL 186	**Aktive Matter I (joint session DY/BP/CPP, organized by DY)**
CPP 45.1–45.8	Wed	15:00–17:15	SCH A251	**Biomaterials and Biopolymers (joint session BP/CPP, organized by BP)**
CPP 46.1–46.8	Wed	15:00–17:00	CHE 91	**Organic Thin Films II (joint session CPP/DS/HL, organized by DS)**
CPP 47.1–47.7	Wed	16:15–18:15	ZEU 255	**Fluids and Interfaces I**
CPP 48.1–48.13	Wed	18:30–21:00	P2-OG1	**Poster: Polymer Crystallization, Nucleation and Selfassembly**
CPP 49.1–49.16	Wed	18:30–21:00	P2-OG1	**Poster: Surfaces, Interfaces, Thin Films, Nanostructures**
CPP 50.1–50.38	Wed	18:30–21:00	P3	**Poster: Organic Electronics and Photovoltaics, Molecular Excitations**
CPP 51.1–51.10	Wed	18:30–21:00	P3	**Poster: Charged Soft Matter, Polyelectrolytes, Ionic Liquids**
CPP 52.1–52.12	Wed	18:30–21:00	P3	**Poster: Hydogels, Microgels, Responsive Polymers**
CPP 53.1–53.1	Thu	9:30–10:00	ZEU 222	**Keynote Lecture III**
CPP 54.1–54.12	Thu	9:30–13:00	HÜL 186	**Active Matter II (joint session DY/BP/CPP, organized by DY)**
CPP 55.1–55.8	Thu	10:15–13:00	ZEU 222	**Focus: Static and Dynamic Disorder Phenomena on the Transport in Organic Semiconductors I**
CPP 56.1–56.9	Thu	10:15–13:00	ZEU 260	**Hydrogels and Microgels I**
CPP 57.1–57.10	Thu	10:15–13:00	ZEU 114	**Thin Films, Nanostructures and Nanoparticles I**
CPP 58.1–58.8	Thu	10:15–12:45	ZEU 255	**Fluids and Interfaces II**
CPP 59.1–59.9	Thu	15:00–18:00	ZEU 222	**Focus: Static and Dynamic Disorder Phenomena on the Transport in Organic Semiconductors II**

CPP 60.1–60.9	Thu	15:00–18:00	ZEU 260	**Focus: Topological Problems in the Physics of Polymers, Biopolymers and Fibers I (joint session BP/CPP, organized by CPP)**
CPP 61.1–61.8	Thu	15:00–17:00	ZEU 114	**Charged Soft Matter, Ionic Liquids and Polyions II**
CPP 62.1–62.12	Thu	15:00–18:15	ZEU 255	**Fluids and Interfaces III**
CPP 63.1–63.1	Fri	9:30–10:00	ZEU 222	**Keynote Lecture IV**
CPP 64.1–64.8	Fri	9:30–11:45	CHE 91	**Organic-Inorganic Hybride Interfaces (joint session CPP/DS/HL, organized by DS)**
CPP 65.1–65.10	Fri	9:30–12:30	HÜL 186	**Complex Fluids and Soft Matter (organized by DY)**
CPP 66.1–66.9	Fri	10:00–12:30	ZEU 118	**Glasses and Glass Transition (joint session DY/CPP/DF, organized by DY)**
CPP 67.1–67.6	Fri	10:15–13:00	ZEU 222	**Focus: Topological Problems in the Physics of Polymers, Biopolymers and Fibers II (joint session BP/CPP, organized by CPP)**
CPP 68.1–68.11	Fri	10:15–13:15	ZEU 260	**Hydrogels and Microgels II**
CPP 69.1–69.10	Fri	10:15–13:00	ZEU 114	**Thin Films, Nanostructures and Nanoparticles II**
CPP 70.1–70.10	Fri	10:15–13:15	ZEU 255	**Organic Electronics and Photovoltaics V: OPV (joint session CPP/DS/HL, organized by CPP)**
CPP 71.1–71.5	Fri	10:30–13:00	HSZ 02	**Frontiers of Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond**

Annual General Meeting of the Chemical and Polymer Physics Division

Thursday 18:30–19:15 ZEU 222

- Bericht
- Wahl des Sprechers
- Verschiedenes

CPP 1: Keynote Lecture I

Time: Monday 9:30–10:00 Location: ZEU 222

Invited Talk CPP 1.1 Mon 9:30 ZEU 222

Dynamically Reconfigurable Soft Matter in External Fields: Smart Particle Gels, Shape-Changing Clusters and Self-Propelling Microbots — •Orlin D Velev — Department of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, NC 27695, USA

This talk will focus on principles of using magnetic and electric fields to manipulate new classes of soft matter assembled from responsive, asymmetric, and motile particles. Metallo-dielectric particles acquire complex polarization patterns in external fields, leading to their multidirectional interactions and assembly. First, we will describe how magnetically responsive Janus microcubes can be assembled into clusters and chains that spontaneously reconfigure when the external magnetic field is turned on and off. The magnetization of the metallic facets leads to directional dipole-dipole and field-dipole interactions. The folding pattern of the clusters is encoded by the orientational sequence of the cubes. Assemblies of specific sequences demonstrate prototypes of new microbot and colloidal origami structures. The dynamically reconfiguring clusters can also be designed to be self-motile in media with non-Newtonian rheology or to serve as microrheometers. In the second part of the talk, we will discuss a new smart gel system of ultra-flexible chains from super-paramagnetic nanoparticles coated by condensed lipid shells. The field collects the nanoparticles into magnetically responsive filaments. The soft, "snappable," capillary interactions also enable the assembly of patchy particles, magnetically self-repairing gel networks and novel inks for 3D printing.

CPP 2: Mechanics and Dynamics of 3D Tissues (joint focus session BP/CPP, organized by BP)

Time: Monday 9:30–13:00 Location: SCH A251

Invited Talk CPP 2.1 Mon 9:30 SCH A251

Cilia-based transport networks — •Eberhard Bodenschatz — MPI für Dynamik und Selbstorganisation , Am Fassberg 17, 37077 Goettingen

Cerebrospinal fluid conveys many physiologically important signaling factors through the ventricular cavities of the brain. We investigated the transport of cerebrospinal fluid in the third ventricle of the mouse brain and discovered a highly organized pattern of cilia modules, which collectively give rise to a network of fluid flows that allows for precise transport within this ventricle. Our work suggests that ciliated epithelia can generate and maintain complex, spatiotemporally regulated flow networks. I shall also show results on how to assemble artificial cilia and cilia carpets. This work is in collaboration with Regina Faubel, Gregor Eichele, Christian Westendorf, Azam Gholami, Isabella Guido, Yong Wang, Albert Bae and Marco Tarantola. Support by the Max Planck Society and the BMBF within the MaxSynBio initiative is gratefully acknowledged.

CPP 2.2 Mon 10:00 SCH A251

Quantitative structure-function relationships in 3D tissues — •Janna Nawroth — Emulate Inc., Boston, MA, USA

Biological tissues are characterized by an organ-specific three-dimensional, multiscale organization of cells and extracellular matrix components. This organization gives rise to organ-specific functions and dysfunctions. Tissue engineering attempts to recapitulate these structure-function relationships in vitro to provide models of disease, drug toxicity, and patient-specific responses. One major challenge is to identify and implement quantitative metrics that capture the most relevant structure-function relationships to serve for both quality control and experimental readout of the engineered tissue. Here, I present engineering and analysis strategies for recapitulating and quantifying the cellular organization and mechanical functions in engineered cardiac muscle and in ciliated epithelia, with a particular emphasis on organ-on-chip technology.

CPP 2.3 Mon 10:30 SCH A251

***In vivo* quantification of spatially-varying mechanical properties in developing tissues** — •Friedhelm Serwane[1,2], Alessandro Mongera[1], Payam Rowghanian[1], David Kealhofer[1], Adam Lucio[1], Zachary Hockenbery[1], and Otger Campas[1] — [1]University of California, Santa Barbara, USA — [2]Max Planck Institute for Medical Research, Heidelberg, Germany

We present a technique that allows quantitative spatiotemporal measurements of mechanical properties *in vivo* using biocompatible ferrofluid droplets as local mechanical actuators [1].

The mechanical properties of the cellular microenvironment and their spatiotemporal variations play a central role in controlling cell behavior, including cell differentiation. However, no direct *in vivo* and *in situ* measurement of mechanical properties within developing 3D tissues has been performed yet.

Using our technique we show that vertebrate body elongation entails spatially varying tissue mechanics along the anteroposterior axis. Specifically, we find that the zebrafish tailbud is viscoelastic: elastic below a few seconds and fluid after just one minute. Furthermore, it displays decreasing stiffness and increasing fluidity towards its posterior elongating region.

This method opens the door to study mechanobiology *in vivo*, both in embryogenesis and in disease processes, including cancer.

[1] F. Serwane, A. Mongera, P. Rowghanian, D. Kealhofer, A. Lucio, Z. Hockenbery, O. Campàs. Nature Methods, in press (2016)

CPP 2.4 Mon 10:45 SCH A251

Mechanical spectroscopy of retina explants at the protein level employing nanostructured scaffolds — •Mareike Zink[1] and S. G. Mayr[2] — [1]Soft Matter Physics Division, University of Leipzig, Leipzig, Germany — [2]Leibniz Institute for Surface Modification (IOM), Leipzig, Germany & Division of Surface Physics, Department of Physics and Earth Sciences, University of Leipzig, Germany

The mechanical properties of the retina play a crucial role in function and diseases of the eye. Here we present that nanostructured TiO2 substrates can be employed as vibrating reed to investigate the mechanical properties of adult mammalian retinae at the nanometer. Within a self-designed mechanical spectroscopy setup, the reed with the retina on top is excited to perform free damped oscillations. The detected oscillation parameters represent a fingerprint of the frequency-dependent mechanical tissue properties that are derived in combination with sandwich beam analysis and finite element calculations. We found that the Young's modulus of the retina is of the order of a few GPa, much higher than values obtained from experiments in which tissue response is investigated on micrometer length scales. In our study, polymers and proteins on the photoreceptor side of the retina in contact with the nanostructured reed are stretched and compressed during vibration of the underlying scaffold and the acting intramolecular forces are probed at the protein level. To this end, our mechanical spectroscopy approach offers new perspectives in studying mechanical response of individual proteins within the tissue for investigating tissue mechanics, diseases and the effect of drugs.

15 min break

CPP 2.5 Mon 11:15 SCH A251

A simulation study on 3D muscle movement: eigen-frequency and force-coupling to the skeleton change with muscle activity — Daniel F B Haeufle, Daniel Wirtz, •Kevin Kraschewski, Syn Schmitt, and Oliver Röhrle — Stuttgart Research Center for Simulation Technology (SimTech), University of Stuttgart, Germany

The muscles in the human body are soft materials coupled flexibly to the rather rigid bones. Due to this flexible coupling, muscles move relative to the bones during movement. The resulting coupling forces of these so-called wobbling masses depend on the neural stimulation of the muscle tissue. It is experimentally very difficult to study the relation between muscle stimulation and coupling forces. Therefore, we developed a 3D continuum-mechanical model of a muscle-tendon complex considering muscle stimulation, elasticity, viscosity, fiber orientation, and tendon stiffness. This model predicts the interaction forces in response to external oscillatory excitations in dependence on excitation frequency and muscle stimulation level. With this approach, the functional role of wobbling masses in human movement, e.g., energy dissipation and force reduction during the impact in human running, can be studied in more detail.

CPP 2.6 Mon 11:45 SCH A251

Electromechanical Turbulence in the Heart — •Jan Christoph and Stefan Luther — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

The self-organizing pattern forming mechanisms underlying highly life-threatening cardiac fibrillation are still insufficiently understood. High-speed fluorescence imaging provides highly detailed visualizations of the spatio-temporal electrophysiological activity of the heart. During ventricular fibrillation, these visualizations depict complex spatio-temporal electrical patterns including rotating vortices or spiral waves on the heart's surface. However, with limited penetration depths of fluorescence imaging the optically mapped surface dynamics reflect only the superficial projection of three-dimensional wave phenomena that evolve within the depths of the cardiac muscle.

We combined fluorescence imaging with ultrasound to study the coupled electrical and mechanical activity of the fibrillating heart on its surface as well as within the heart wall. We found that during fibrillation electrical activity patterns and elasto-mechanical deformations are highly correlated producing co-localized patterns of electrical and mechanical activation. Specifically, we found that electrical spiral wave rotors can be accompanied by rotational elasto-mechanical patterns, which like fingerprints of vortex activity occur as a characteristic feature within the deformations of the fibrillating muscle. Our data highlights the importance of studying the mechanics and dynamics of 3D cardiac tissues to obtain a better understanding of cardiac arrhythmias and to conceptualize novel diagnostic and therapeutical strategies.

CPP 2.7 Mon 12:00 SCH A251

Local rules for robust global transport in liver networks — •Jens Karschau[1], Andre Scholich[2], Marius Asal[1], Hidenori Nonaka[3], Hernan Morales-Navarrete[3], Fabian S Miranda[3], Kirstin Meyer[3], Yannis Kalaidzidis[3], Marino Zerial[3], Frank Jülicher[2], and Benjamin M Friedrich[1] — [1]cfaed / TU Dresden — [2]MPI PKS, Dresden — [3]MPI CBG, Dresden

The liver represents a chemical factory that is characterised by intertwined transport networks for toxins and metabolites. Each hepatocyte cell of the liver tissue interacts with two space-filling networks: bile canaliculi and sinusoids which transport bile and blood, respectively. How these networks establish their distinct architecture to supply all hepatocytes, and dynamically adapt to time-varying load as well as to local perturbations remains elusive.

Here, we elucidate design principles of liver tissue structure and self-organisation based on experimental high-resolution imaging data from mice. First, we characterise and quantify liver tissue with tools from liquid-crystal theory that show lobule level patterns of aligned cell polarity and local network anisotropy. Second, we study a simplified flow model to understand the relationship between the spatial structure of the network and robust transport properties. Third, we compare our flow simulations in reconstructed bile canaliculi networks and simulated self-organised networks. Thereby, we establish a connection between local network geometry and properties of global fluid transport, linking tissue structure with function.

CPP 2.8 Mon 12:15 SCH A251

Jamming and liquidity in 3D cancer cell aggregates — •Linda Oswald[1], Steffen Grosser[1], Jürgen Lippoldt[1], Steve Pawlizak[1], Anatol Fritsch[2], and Josef Käs[1] — [1]University of Leipzig — [2]MPI CBG Dresden

Traditionally, tissues are treated as simple liquids, which holds for example for embryonic tissue. However, recent experiments have shown that this picture is insufficient for other tissue types, suggesting possible transitions to solid-like behavior induced by cellular jamming. The coarse-grained self-propelled Voronoi (SPV) model predicts such a transition depending on cell shape which is thought to arise from an interplay of cell-cell adhesion and cortical tension. We observe non-liquid behavior in 3D breast cancer spheroids of varying metastatic potential and correlate single cell shapes, single cell dynamics and collective dynamic behavior of fusion and segregation experiments via the SPV model.

CPP 2.9 Mon 12:30 SCH A251

Type IV pili govern the internal dynamics of *Neisseria gonorrhoeae* microcolonies. — •Wolfram Pönisch[1], Christoph Weber[2], Khaled Alzurqa[3], Hadi Nasrollahi[3], Kelly Eckenrode[3], Nicolas Biais[3], and Zaburdaev Vasily[1] — [1]Max Planck Institut für Physik Komplexer Systeme, Dresden — [2]Harvard University, Cambridge — [3]Brooklyn College, New York

An important step in the evolution of biofilms is the formation of microcolonies, agglomerates of cells that can consists of several thousands of cells. For many pathogenic bacteria, i.e. *N. gonorrhoeae* or *P. aeruginosa*, the attractive cell-cell-interactions required for microcolonies to form are mediated by micron-long and thin appendages, the called type IV pili. We are interested in the pili-mediated dynamics of individual bacteria within microcolonies and how they affect the properties of the agglomerates. In experiments, we observe a gradient of motility of cells of *N. gonorrhoeae*, depending on their position within a colony. We will present a computational model of cells interacting via individual pili. It allows us to model microcolonies on biologically relevant temporal and spatial scales and is able to reproduce the differential motility of cells within a colony. Furthermore, it enables us to study quantities that are not yet accessible by experiments, e.g. the cell density within a colony, the pili-mediated cell forces and force fluctuations and the internal structure of the colonies. Finally, we will present how the assembly and morphology of microcolonies is affected by the pili properties, particularly for mixtures of cell populations characterized by mutations of their pilus apparatus.

CPP 2.10 Mon 12:45 SCH A251

Growth Dynamics of Biofilms — •Benedikt Sabass[1,2], Jing Yan[2], Howard A. Stone[2], and Ned S. Wingreen[2] — [1]Forschungszentrum Jülich — [2]Princeton University

Bacteria can form tight communities that are called biofilms. Although biofilms are ubiquitous and ecologically important, little is known about the physics of biofilm growth. Here, we focus on rod-shaped V. cholerae bacteria that form hemispherical biofilms when growing on a surface. Using high-resolution microscopy data, we measure cell density, cell orientation, and shape evolution of the biofilm. We quantitatively explain the density and cell orientation inside the biofilm by minimization of elastic energies. The evolution of the whole biofilm shape is governed by apparent viscous relaxation. We find that the shape parameters of biofilms follow rather simple, generic scaling laws.

CPP 3: Fundamentals of Perovskite Photovoltaics I (joint session CPP/DS/HL)

Time: Monday 10:15–13:00 Location: ZEU 222

Invited Talk CPP 3.1 Mon 10:15 ZEU 222

The Versatility of Mesoscopic Solar Cells — •Anders Hagfeldt — Laboratory of Photomolecular Science, Swiss Federal Institute of Technology Lausanne (EPFL), CH-1015, Lausanne, Switzerland

In our work on solid-state dye-sensitized solar cells (ssDSSC) we have recently [1] shown that copper phenanthroline complexes can act as an efficient hole transporting material, achieving power conversion efficiencies of more than 11%.

In our work on perovskite solar cells (PSC) we have achieved efficiencies above 20% with a mixed composition of iodide/bromide and methyl ammonium/formamidinium. With the use of SnO2 compact underlayers as electron acceptor contacts we have constructed planar perovskite solar cells with a hysteresis free efficiency above 20% [2]. We have taken the cation mixing of the perovskite film further by including Cs+ and Rb+. Larger grains grown in a monolithic manner are observed and for example reproducibility and device stability are improved [3]. At the meeting we will discuss our champion data; up to 22% efficiency with an external electroluminescence of 4%, and an outstanding open-circuit voltage of 1.24 V at a band gap of 1.63 eV. Furthermore, we will report a breakthrough in stability at 85 oC for 500 h under full solar illumination.

References [1]*Freitag et al., Energy & Envir. Sci., DOI: 10.1039/C5EE1204J [2]*Correa et al., Energy & Envir. Sci., DOI:10.1039/C5EE02608C [3]*M. Saliba et al., Science 10.1126/science.aah5557 (2016)

CPP 3.2 Mon 10:45 ZEU 222

Impact of Preparation Conditions on Properties of Perovskite Thin Films — •Alexander Hinderhofer[1], M. Ibrahim Dar[2], Jan Hagenlocher[1], Neha Arora[2], Michael Grätzel[2], and Frank Schreiber[1] — [1]Institute of Applied Physics, University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — [2]Laboratory of Photonics and Interfaces, EPFL, CH-1015 Lausanne, Switzerland

The performance of light emitting and light harnessing perovskite thin film devices depend strongly on their structural features. The so-called two-step conversion for preparing perovskite thin films, involves the deposition of lead halide precursor onto a substrate and the subsequent transformation of the resulting films into the perovskite phase by spin coating (drop casting) or dipping into an isopropanol solution containing a defined amount of methylammonium halide (CH_3NH_3X) (X=I,Br). It is well-known that the morphology and structural properties of perovskite depend strongly on the exact preparation conditions.

We applied grazing incidence wide angle x-ray scattering (GIWAXS) to determine the domain size and preferred orientation in several perovskite thin films. We will discuss the impact of different solvents and preparation methods (spin coating, dip coating) on the structure and morphology of the different perovskite films and we comment on the device performance. Finally, we will comment on the time scale of the crystallization process in $CH_3NH_3PbI_3$ perovskite thin films, which is accessible by in situ real time x-ray scattering.

CPP 3.3 Mon 11:00 ZEU 222

Analysis of electronic trap states in methylammonium lead halide perovskite solar cells via thermally stimulated current — •Philipp Rieder[1], David Kiermasch[1], Mathias Fischer[1], Kristofer Tvingstedt[1], Andreas Baumann[1,2], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research ZAE, 97074 Würzburg

While power conversion efficiencies already exceeding 22% have been achieved for organo lead halide perovskite solar cells, a complete understanding of its fundamental working principles is still missing, but nonetheless essential to further improve this type of thin film photovoltaic. To address the impact of electronic trap states on device performance, we probed solution processed methylammonium lead halide perovskite solar cells via thermally stimulated current (TSC) analysis. Thereby, after cooling the sample down to 10 K, possible trap states are filled optically and gradually released again by heating the sample back up to 300 K. This causes a weak current to flow, which allows to draw conclusions about the trap state density as well its energetic depth. We probed perovskite solar cells in normal as well as inverted device configuration to identify the influence of different transport layers on the energetic trap landscape and observe a substantial addition in the case of the commonly used TiO_2. Additionally, we studied the effect of incorporating bromine as well as chlorine to partly replace the iodine on the electrically active trap state distribution of the photoactive semiconductor.

CPP 3.4 Mon 11:15 ZEU 222

Strong impact of processing parameters on morphology and crystal orientation of hybrid perovskite thin films for photovoltaic application — •Johannes Schlipf[1], Lukas Oesinghaus[1], Yinghong Hu[2], Nadja Giesbrecht[2], Sigrid Bernstorff[3], Thomas Bein[2], Pablo Docampo[4], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]Department of Chemistry and CENS, LMU München, 80539 München — [3]Elettra-Sincrotrone Trieste S.C.p.A., Basovizza, 34149 Trieste, Italy — [4]Newcastle University, School of Electrical and Electronic Engineering, Newcastle upon Tyne NE1 7RU, UK

After five years of rapid research, power conversion efficiencies of hybrid perovskite solar cells (PSC) around 20% have become feasible for solution-processed multicrystalline thin films. However, photovoltaic performance, reproducibility and stability of PSC devices depend on crystal size and orientation which in turn are affected by processing parameters during synthesis. We investigate hybrid perovskite thin films with small and wide angle X-ray scattering (GISAXS, GIWAXS) and thereby identify key crystallization mechanisms that strongly influence film morphology and crystal orientation [1,2]. This not only shows the importance of rigorous control of processing parameters, but also renders film morphologies tunable which allows for a rational development of new synthesis methods for high efficiency PSC. [1] J. Schlipf et al., J. Phys. Chem. Lett. 2015, 6, 1265. [2] L. Oesinghaus et al., Adv. Mater. Interfaces 2016, 1600403.

15 min break

CPP 3.5 Mon 11:45 ZEU 222

Local Time-Dependent Charging in a Perovskite Solar Cell — Victor W. Bergmann[1], Ilka M. Hermes[1], Dan Li[1], Alexander Klasen[1], Simon Bretschneider[1], Eiichi Nakamura[2], Rüdiger Berger[1], and •Stefan A.L. Weber[1,3] — [1]Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [2]The University of Tokyo, Tokyo 113-0033, Japan — [3]Johannes Gutenberg University Mainz, 55128 Mainz, Germany

Efficient charge extraction within solar cells explicitly depends on the optimization of the internal interfaces. Potential barriers, unbalanced charge extraction or interfacial trap states can prevent cells from reaching high power conversion efficiencies. Furthermore, in perovskite solar cells, slow processes happening on timescales of seconds cause hysteresis. Here, we report on local and time-dependent potential measurements with Kelvin probe force microscopy (KPFM) on cross sections [1] of planar methylammonium lead iodide (MAPI) perovskite solar cells. The KPFM revealed distinct differences in the charging dynamics at interfaces of the MAPI to adjacent layers [2]. Illumination experiments showed that more than one process is involved in hysteresis. By locally resolving these processes we found distinct differences in the charging dynamics in different regions of the device. Our results support the scenario of mobile ions and interfacial trap states for explaining the hysteresis in our device. [1] Nat. Commun. 2014, 5. [2] ACS Appl. Mater. Interfaces, 2016, 8 (30), 19402.

CPP 3.6 Mon 12:00 ZEU 222

Effect of Thermal and Structural disorder on Electronic Structure in Methylammonium Lead Halide Perovskites — •Cheng Li[1], Shivam Singh[2], Fabian Panzer[3], K L. Narasimhan[2], Yu Zhong[1], Anna Gräser[1], Tanaji Gujar[1], Mukundan Thelakkat[1], Anna Köhler[3], Dinesh Kabra[2], and Sven Huettner[1] — [1]Macromolecular Chemistry I, Universität Bayreuth, Universitätstr. 30, 95447 Bayreuth, Germany — [2]Indian Institute of Technology Bombay, Powai, 400076 Mumbai, Indian — [3]Experimentalphysik II, Universität Bayreuth, Universitätstr. 30, 95447 Bayreuth, Germany

In this work, to understand the structure of perovskite materials, we investigate the temperature dependence of optical properties of perovskite from room temperature (300K) to 6K. Unlike typical inorganic semiconductor, in both tetragonal (T>163K) and orthorhombic (T<163K) phases of MAPbI3, the band gap decreases with decrease in temperature. We indicate that this temperature dependence of the band gap is governed by the lattice expansion term instead of the electron-phonon interaction. The exciton linewidth is homogeneously broadened in both phases. The absorption, at the low energy edge of the exciton absorption, increases exponentially with energy, i.e reminiscent of Urbach tail absorption. The Urbach energy which is used to characterize order of structure, is modelled using thermal and static disorder for both phases separately.This work provides important insights to the electronic and structural properties of MAPbI3 based perovskites, and this method is transferable to many related perovskites.

CPP 3.7 Mon 12:15 ZEU 222

Impact of bromine doping on recombination kinetics in perovskite solar cells — •David Kiermasch[1], Phillip Rieder[1], Kristofer Tvingstedt[1], Andreas Baumann[2], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern) Bayern, 97074 Würzburg

Organo metal halide perovskite solar cells exhibit exceptionally good power conversion efficiency values exceeding already 20%. To allow further improvements it is important to understand the limiting processes e.g. charge carrier recombination in this new photovoltaic technology. Most of the recombination studies presented so far have been focused on perovskite films or crystals but only a few have studied the charge carrier dynamics in solar cell devices. We report on charge carrier lifetime values in bromine containing planar perovskite solar cells with varying the bromine content. The lifetime and corresponding charge carrier density has been derived from transient photovoltage (TPV) and charge carrier extraction (CE) experiments. We found increased lifetime values in solar cells with bromine ($\mathrm{MAPb(I_{3-x}Br_x)_3}$) compared to pure methylammonium lead iodine ($\mathrm{MAPbI_3}$). Furthermore, the CE signals from the bromine containing solar cells can be divided in two different extraction parts on different time scales leading to anomalously high extracted charge values. We discuss the experimental findings in regard of possible different contributions to the CE signal.

CPP 3.8 Mon 12:30 ZEU 222

Reduced Recombination for High-Open-Circuit Voltages in CH3NH3PbI3 Solar Cells — •Christian M. Wolff[1], Fengshuo Zu[2], Andreas Paulke[1], Lorena Perdigon Toro[1], Norbert Koch[2], and Dieter Neher[1] — [1]Universität Potsdam, Institut für Physik und Astronomie — [2]Humboldt-Universität zu Berlin, Institut für Physik

Perovskite solar cells with all-organic transport layers have shown efficiencies rivalling their counterparts that employ inorganic transport layers while avoiding high temperature processing. We investigate how the choice of the fullerene derivative employed in the electron-transporting layer of inverted perovskite cells affects the open circuit voltage. Non-radiative recombination mediated by the electron-transporting layer is the determining factor for the open-circuit voltages in our cells. By inserting an ultra thin layer of an insulating polymer between the active CH3NH3PbI3 perovskite and the fullerene layer, external radiative efficiencies of up to 0.3%, open-circuit voltages (Voc) as high as 1.16V and with efficiencies up to 19.4% were realised. Our results show that reduction of non-radiative recombination due to charge-blocking at the perovskite/organic interface is more important than proper alignment in the search for ideal selective contacts for high Voc.

CPP 3.9 Mon 12:45 ZEU 222

On the chemical origins of crystalline preferred orientations in hybrid organometallic lead halide perovskite thin films — •Shambhavi Pratap, Johannes Schlipf, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Solar cells based on organometallic lead halide perovskites have established themselves as a promising alternative to commercial thin film solar cells. The crystallographic versatility of the material allows the possibility of extensive chemical tuning, which manifests in the material as a spectra of properties that may be obtained. This entices research on hybrid perovskite structures combining different organic and inorganic groups into a crystalline framework. Preferential orientations of the crystalline hybrid perovskites (1) are reported and correlated to their morphological and chemical characteristics by grazing incidence wide angle x-ray scattering (GIWAXS). Remarkably, perovskite thin films prepared by the same methodologies displayed varying behaviors of preferred orientations, as their chemical composition was varied. Moreover, the route and rate of crystallization (2) is known to radically influence crystalline preferred orientations as well, giving rise to information regarding kinetic and thermodynamic orientations. These results, for the first time propose the possibility of controlling crystallinity of spin-coated thin films by tuning the ingredients of and the treatment of the solution used for spin coating.

(1) Oesinghaus et al., Adv. Mater. Interfaces 2016, 3, 1600403
(2) Giesbrech et al., ACS Energy Lett. 2016, 1, 150-154

CPP 4: Bioinspired Functional Materials I

Time: Monday 10:15–13:00 Location: ZEU 114

Invited Talk CPP 4.1 Mon 10:15 ZEU 114

Membrane nanotube formation in giant vesicles — •Rumiana Dimova — Max Planck Institute of Colloids and Interfaces, Science Park Golm, 14424 Potsdam, Germany

Nanotubes are ubiquitous in cells. Examples for tubular structures are provided not only by organelles such as the Golgi body and the endoplasmic reticulum but also by intercellular connections between different cells. Their geometry and large area-to-volume ratio make them an excellent natural tool for membrane storage, sorting and transport. Such nanotubes can also be formed from synthetic lipid bilayers. Here, we discuss two systems based on giant vesicles, within which lipid nanotubes are generated and stabilized by spontaneous curvature. In the first case, we employ membranes doped with the ganglioside GM1 (Biophys. J. 111:1935, 2016). Upon dilution, the vesicle membrane exhibits asymmetric composition set by the different surface GM1 coverage on the two membrane leaflets. Employing vesicle micromanipulation and electroporation, we could assess the GM1 asymmetry and the associated spontaneous curvature. In the second system, the two leaflets of the bilayer have the same composition, but the solutions in contact with the inner and outer leaflet differ in the concentration of polyethylene glycol (PEG). We show that the spontaneous curvature is now generated by weak adsorption of PEG onto the membranes (ACS Nano 10:463, 2016). The tube shapes, cylindrical or necklace-like, and their diameters can be varied by the membrane composition and bending rigidity. We demonstrate this variation by employing membranes in the liquid-ordered and liquid-disordered phase state.

CPP 4.2 Mon 10:45 ZEU 114

Traction forces of water droplets on superhydrophobic pillar structures — •Schellenberger Frank, Saal Alexander, and Tress Martin — Max Planck Institute for Polymer Research, Mainz, Germany

Surfaces with super-hydrophobic properties play an important role in both nature and science. Thereby, the artificial surfaces typically try to copy the characteristic features of their natural pendants. That is in general, a hydrophobic surface chemistry combined with a structured topography. To investigate the particular impact of these characteristics model surfaces with pillars of varying size, arrangement and surface coating have been employed [1]. While many studies used rigid pillars to maintain a well-defined topography, in the present work flexible pillars are focused. When imaged with a Laser Scanning Confocal Microscope, these flexible pillars act as cantilevers to detect traction forces of a drop resting on their top. By that, the distribution of the forces in parallel to the surface along the contact line is recorded. Especially the traction forces of the receding contact line of an evaporating or advancing drop will be illuminated.

[1] P. Papadopoulos et al. PNAS 9 (2013) 3254

CPP 4.3 Mon 11:00 ZEU 114

Functional biohybrid materials: Centric diatoms with incorporated donor-acceptor laser dye couples — Lukas Selzer, Michael Grimann, and •Thomas Fuhrmann-Lieker — University of Kassel, Institute of Chemistry and Center for Interdisciplinary Nanostructure Science and Technology, 34109 Kassel, Germany

Centric diatoms are unicellular algae with an intricate cell wall of silica that can be described as a photonic crystal slab waveguide. The photonic function can be enhanced by the incorporation of laser dyes, turning the living algae into active fluorescent light-emitters. In order to increase the photoluminescence efficiency, we achieved dual in-vivo-staining with a dye pair for fluorescence resonant energy transfer (FRET). In addition to applications in photonics, this method allows the determination of the acceptor dye concentration in the hybrid material.

CPP 4.4 Mon 11:15 ZEU 114

DNA based assembly of plasmonic nanoantennas — •Mathias Lakatos[1], Hanna Brunner[1], Darius Pohl[2], Andreas Heerwig[1], Bernd Rellinghaus[2] und Michael Mertig[1] — [1]TU Dresden, Physikalische Chemie, Mess- und Sensortechnik, 01062, Dresden — [2]IFW, Institut für Metallische Materialien, 01171 Dresden

Based on the ability of DNA to self-assemble into complex 2D and 3D structures with defined dimensions and structure specification at the nanometer scale, optical active nanostructures were synthesized and characterized. The preparation of the DNA template structures was done according to the so-called DNA origami method, where a long single-stranded DNA, the scaffold strand, is folded into a previously designed form by short single-stranded oligonucleotides. The incorporation of specific binding sites enables the local positioning of functional elements. For the construction of plasmonic active nanoantennas, complementary functionalized AuNR were used. Depending on the DNA template structures and the gold nanoparticles, nanoantennas of about 100 nm up to 300 nm size have been realized. Low-loss electron energy loss spectroscopy measurements were carried out using monochromated scanning transmission electron microscopy (STEM) on individual structural elements to gain insight into the localization of different plasmonic modes.

15 min break

CPP 4.5 Mon 11:45 ZEU 114

Vesicles-on-a-chip : A universal microfluidic platform for the assembly of liposomes and polymersomes — •Julien Petit[1], Ingmar Polenz[1], Laura Thomi[2], Frederik Wurm[2], Jean-Christophe Baret[3], Katharina Landfester[2], Stephan Herminghaus[1], and Oliver Bäumchen[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPI-DS), 37077 Göttingen, Germany — [2]Max Planck Institute for Polymer Research (MPI-P), 55128 Mainz, Germany — [3]Centre de Recherche Paul Pascal (CRPP), CNRS, Université de Bordeaux, 33600 Pessac, France

One key challenge nowadays for a "bottom-up" approach in synthetic biology relies on the fabrication of compartments such as vesicles that can be viewed as model membranes. Nevertheless, the development of reliable methods for the high-throughput production of vesicles in an easy and well-controlled manner is still in progress. In this context, we propose a versatile method for producing monodisperse liposomes as well as polymersomes on the exact same PDMS-based microfluidic platform from double-emulsions [J. Petit et al., EPJE 39: 59 (2016)]. The size of the vesicles obtained with this technique can be varied over at least one order of magnitude and they are stable for more than 3 months under ambient conditions. Furthermore, we demonstrate the versatility of this microfluidic platform by producing polymersomes composed of functionalized block-copolymers. We characterize the successful functionalization by fluorescent labeling and measure the specific adhesion of polymersomes on dedicated surfaces using a micropipette force sensor technique.

CPP 4.6 Mon 12:00 ZEU 114

Passive Polymer Translocation Through Membranes: An Edwards Model Based Guideline — •Marco Werner[1,2], Jasper Bathmann[3], Vladimir Baulin[1], and Jens-Uwe Sommer[2] — [1]Universitat Rovira i Virgili, Tarragona, Spain — [2]Leibniz-Institut für Polymerforschung Dresden, Dresden, Germany — [3]Technische Universität Dresden, Dresden, Germany

We propose a theoretical framework for examining translocation of flexible polymers through amphiphilic membranes: A generic model for monomer-membrane interactions is formulated and the Edwards equation is employed for calculating the free energy landscape of a polymer in a membrane environment. By the example of homopolymers it is demonstrated that polymer adsorption and the symmetry of conformations with respect to the membrane's mid-plane trigger passive polymer translocation in a narrow window of polymer hydrophobicity. We demonstrate that globular conformations can be taken into account by means of a screening of the external potential, which leads to excellent agreement of predicted translocation times with dynamic lattice Monte Carlo (MC) simulations. The work opens a theoretical road-map on how to design translocating flexible polymers by referring to universal phenomena only: adsorption and conformational symmetry. As confirmed by MC simulations on amphiphilic polymers, promising candidates of translocating polymers in practice are short-block amphiphilic copolymers, which in the limit of small block sizes resemble homopolymers on a coarse grained level.

CPP 4.7 Mon 12:15 ZEU 114

The Bicontinuous Gyroid-Phase in Purely Entropic Self-Assembly of Hard Pears — •Philipp Schönhöfer[1,2], Laurence Ellison[3], Matthieu Marechal[2], Douglas Cleaver[3], and Gerd Schröder-Turk[1] — [1]School of Engineering and Information Technology, Murdoch University, Murdoch, Australia — [2]Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Erlangen, Germany — [3]Materials and Engineering Research Institute, Sheffield Hallam University, Sheffield, UK

We investigate a model of tapered hard particles reminiscent of pears forming the bicontinuous Ia3d structure by entropic self assembly. Based on the observations of Barmes et al. and Ellison et al. a phase diagram for particles with an aspect ratio $k = 3$ in relation to the degree of tapering k_θ and the tapering angle $\theta = 2\arctan(\frac{1}{2k_\theta})$, respectively, around the gyroid phase is generated. Additionally, the mechanism of interdigitating sheets of pears in these systems to create surfaces with negative Gauss curvature, which is needed to form the gyroid minimal surface is investigated in detail. We show that this mechanism differs from systems, which occur in nature (lipid bilayers) and synthesized materials (di-block copolymers) and where the formation of the gyroid is energetically driven, as for single hard pears do not follow Steiner*s theorem. This behaviour is investigated by Voronoi tessellation, whereas both shape and volume of the Voronoi cells in regard to the gauss curvature of the gyroid surface is determined.

[1] F. Barmes et al., Phys. Rev. E 68, 021708 (2003)

[2] Ellison et al., Phys. Rev. Lett. 97, 237801 (2006)

CPP 4.8 Mon 12:30 ZEU 114

Probing Adhesion with Mechano-Responsive Polymers — •Jens W. Neubauer[1], Longjian Xue[2], Johann Erath[3], Dirk-M. Drotlef[4], Aránzazu del Campo[5], and Andreas Fery[1,6] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Germany — [2]Wuhan University, China — [3]University of Bayreuth, Germany — [4]Max-Planck-Institut für Polymerforschung, Mainz, Germany — [5]Leibniz-Institut für Neue Materialien, Saarbrücken, Germany — [6]Technische Universität Dresden, Germany

We use mechano-responsive polymers to elucidate adhesion. In gecko-inspired micropillar adhesives, for instance, a significant impact of the pillar contact geometry on the adhesion was found. Fundamental differences in their contact stress distributions were predicted by theory. We applied a mechano-responsive polyelectrolyte brush to determine the contact stress distributions of the micropillars. The mechano-response is based on the quenching of a labeled dye so that local tensile and compressive stresses affect the local fluorescence intensity. It was read out with high spatial resolution utilizing confocal laser scanning microscopy.

J.W. Neubauer, L. Xue, J. Erath, D.-M. Drotlef, A. del Campo, A. Fery *ACS Appl. Mater. Interfaces* **8** (2016), 17870-17877.

CPP 4.9 Mon 12:45 ZEU 114

Theoretical quantification of nano carrier loading and release rates — •Richard Schwarzl[1], Fang Du[2], Rainer Haag[2], and Roland R. Netz[1] — [1]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin — [2]Freie Universität Berlin, Institut für Chemie und Biochemie, Arnimallee 14, 14195 Berlin

Macromolecular nanostructures that are used as drug carriers are characterized by their loading and release kinetics. Release studies commonly employ the dialysis method, in which a cellulose membrane separates the solution of released drug from the nanocarrier solution. In order to extract the nano carrier release rate, it is necessary to take the effect of the dialysis membrane on the release kinetics into account. Using a theoretical two-step approach, consisting of the analysis of a calibration experiment of drug diffusion through the dialysis membrane in the absence of nanocarriers, and of an experiment in the presence of nanocarriers, one is able to determine all kinetic rates and in particular to disentangle kinetic dialysis membrane properties from kinetic nanocarrier properties.

CPP 5: Polymer Networks and Dynamics I: Elastomers and Magnetic Materials

Time: Monday 10:15–13:00 Location: ZEU 255

Invited Talk CPP 5.1 Mon 10:15 ZEU 255

A Combined Rheological and Dielectric Analysis of Filler Networking in Elastomer Nano-Composites — •Manfred Klüppel — Deutsches Institut für Kautschuktechnologie e.V., Eupener Str. 33, D-30519 Hannover, Germany

The dynamics of filler networking (flocculation) in carbon black filled elastomer composites is investigated by dielectric relaxation spectroscopy during oscillatory shearing in a plate-plate rheometer. It is demonstrated that during heat treatment at low strain amplitude, a pronounced filler networking takes place in rubber melts leading to a simultaneous increase of the shear modulus and dc-conductivity. Two relaxation times, obtained from a Cole-Cole fit of the dielectric spectra, are identified, which both decrease strongly with increasing flocculation time. This behavior is analyzed in the frame of fractal network models. During filler networking, a universal scaling behavior holds between the conductivity and the corresponding high frequency relaxation time, which fits all the measured data. It is demonstrated that the underlying basic mechanism is a change of the correlation length of the filler network, i.e. the size of the fractal heterogeneities. This decreases during filler networking due to the formation of additional conductive paths. The same universal scaling behavior is found for temperature dependent dielectric measurements of the cured systems, which are heated from room temperature up to 200 °C. Thereby, the conductivity decreases and the relaxation time increases, indicating that the filler network breaks up randomly due to the thermal expansion of the rubber matrix.

CPP 5.2 Mon 10:45 ZEU 255

Investigation of strain induced crystallization of natural rubber under cyclic impact loading — •Konrad Schneider — Leibniz-Institut für Polymerforschung Dresden, Hohe Str. 6, 01069 Dresden, Germany

Strain induced crystallization (SIC) is one of the special features of natural rubber (NR), responsible for its outstanding mechanical performance. Nevertheless, for short term behaviour of NR, e.g. within a rolling tire, the dynamic of SIC plays an important role. By means of synchrotron x-ray scattering SIC is monitored during impact loading together with recording energy dissipation by thermography. The results enable a more realistic modelling of the dynamic behaviour of natural rubber.

CPP 5.3 Mon 11:00 ZEU 255

Nano-mechanical imaging reveals heterogeneous cross-link distribution in sulfur-vulcanized butadiene-styrene rubber comprising ZnO particles — Yulia Glebova[1,2], •Valentin Reiter-Scherer[1], Sari Suvanto[3], Tarmo Korpela[3], Tuula T. Pakkanen[3], Nikolai Serverin[1], Vladimir Shershnev[2], and Jürgen P. Rabe[1] — [1]Department of Physics and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany — [2]Moscow State University of Fine Chemical Technologies, Russia — [3]Department of Chemistry, University of Eastern Finnland, Finnland

The addition of zinc oxide (ZnO) to sulfur (S-) vulcanized rubbers is known to accelerate the cross-linking kinetics and to increase the heterogeneity of the cross-link density. However, the spatial distribution of cross-links is hardly known and the mechanism of the activity of ZnO is disputed. We therefore investigated S-vulcanized butadiene-styrene rubber comprising ZnO particles. The samples were fractured and then investigated employing the nano-mechanical mapping mode (NM) of scanning force microscopy (SFM), supported by scanning electron microscopy (SEM). We find that rubber around the ZnO particles exhibits a higher Young's modulus in a shell with a width up to about 200 nm. Furthermore, the extension and retraction curves on these shells exhibit a smaller hysteresis than on the rubber further away from the ZnO particles. We attribute the higher Young's modulus and the smaller hysteresis to a higher cross-link density in rubber surrounding the ZnO particles and we discuss a mechanism of the activity of ZnO in rubbers which can explain this.

CPP 5.4 Mon 11:15 ZEU 255

Force-induced matrix-mediated interactions between rigid inclusions in elastic media — Mate Puljiz[1], Shilin Huang[2], Günter K. Auernhammer[2], and •Andreas M. Menzel[1] — [1]Heinrich Heine University Düsseldorf, Düsseldorf, Germany — [2]Max Planck Institute for Polymer Research, Mainz, Germany

The situation of forces acting on rigid inclusions in elastic matrix environments is addressed. These forces can be imposed from outside, or they are induced between the inclusions, if, for example, external electric or magnetic fields generate interacting electric or magnetic moments in the inclusions. Resulting translations of the inclusions distort the embedding elastic matrix, which gives rise to long-ranged matrix-mediated interactions between the inclusions.

We demonstrate that these induced interactions can be calculated analytically in the case of rigid spherical inclusions [1]. For this purpose, a formalism used to capture hydrodynamic interactions between particles in colloidal suspensions [2] is adapted to the situation of an elastic environment. Experiments on rigid magnetic particles in a soft elastic gel matrix confirm our approach [1]. The description is readily extended to include induced torques [3].

Our results will be important in the future to characterize, for instance, the external tunability of mechanical properties in electric or magnetic composite materials, and for microrheological applications.

[1] Puljiz et al., *Phys. Rev. Lett.* (accepted, 2016).
[2] Dhont, *An Introduction to Dynamics of Colloids* (Elsevier, 1996).
[3] Puljiz et al., *arXiv preprint* arXiv:1611.08823 (2016).

CPP 5.5 Mon 11:30 ZEU 255

Cyclic adjustable nanometer sized ion tracks in Polydimethylsiloxane — •Calvin Brett[1,2,3], Wiebke Ohm[1], Matthias Schwartzkopf[1], Pablo Mota-Santiago[2], Daniel Severin[4], Nigel Kirby[5], Christina Trautmann[4,6], Patrick Kluth[2], Michael A. Ruebhausen[3], and Stephan V. Roth[1,7] — [1]DESY, Notkestr. 85, D-22607 Hamburg — [2]Australian National University, Canberra, ACT 2601 — [3]University of Hamburg, Luruper Chaussee 149, 22761 Hamburg — [4]GSI Helmholtzzentrum für Schwerionenforschung, Planckstraße 1, 64291 Darmstadt — [5]Australian Synchrotron, 800 Blackburn Road, Clayton — [6]Technische Universität Darmstadt, Alarich-Weiss-Straße 2, 64287 Darmstadt — [7]KTH, Teknikringen 56-58, SE-100 44 Stockholm

The efficiency of miniaturization crucially relies on the ability to tailor complex systems on the nanoscale. We used swift heavy ion irradiation as a tool to yield highly controllable nanometer sized features. Hence, we studied the structure and morphology of irradiated Polydimethylsiloxane (PDMS) thin films by means of small angle x-ray scattering (SAXS) and infrared spectroscopy. We found first evidence of ion tracks in silicon based polymers. Furthermore, in situ stretching experiments using SAXS show the appearance of cyclic elastically deformable ion tracks in PDMS. This offers adjustable nanostructures for new applications.

15 min break

CPP 5.6 Mon 12:00 ZEU 255

Switchable nonlinear stress-strain properties and dynamic behavior of magnetic gels — Peet Cremer, Giorgio Pessot, Hartmut Löwen, and •Andreas M. Menzel — Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany

Magnetic gels, ferrogels, and magnetorheological elastomers consist of magnetic colloidal particles embedded in a permanently crosslinked, possibly swollen, elastic polymer matrix. Many of their material properties can be reversibly switched from outside using magnetic fields.

Two of such switchable features are presented and analyzed. First, these are nonlinear stress-strain properties of materials containing chain-like particle aggregates [1,2]. We had previously identified intermediate plateau-like regimes on the stress-strain curves that are tunable by external magnetic fields [1]. Now, we report on the effect of different magneto-mechanical couplings between the magnetic moments and the elastic matrix that qualitatively influence the overall behavior [2]. Second, we determine linear dynamic properties, starting from mesoscopic particle-based models [3]. We analyze the influence of different particle arrangements and magnetic interactions on the linear dynamic storage and loss moduli. Depending on the frequency of the stimulus, qualitatively different trends are observed.

Both aspects are important for the application of magnetorheological gels and elastomers, e.g., as soft actuators or tunable dampers.

[1] Cremer et al., *Appl. Phys. Lett.* **107**, 171903 (2015).
[2] Cremer et al., *Phys. Chem. Chem. Phys.* **18**, 26670 (2016).
[3] Pessot et al., *J. Chem. Phys.* **145**, 104904 (2016).

CPP 5.7 Mon 12:15 ZEU 255

The Dipolar Mean Field Model: A promising Ansatz to describe Magneto-Sensitive Elastomers — •Dirk Romeis and Marina Saphiannikova — Leibniz-Institut für Polymerforschung Dresden e.V., D-01069 Dresden, Germany

Magneto-sensitive elastomers are composed of magnetizable microparticles embedded into a soft-elastic polymer network. In the presence of an external magnetic field these composites can change their mechanical properties significantly. The precise relations and conditions responsible for the actual changes are not fully understood, neither experimentally nor theoretically. Recently, we developed a dipolar mean field approach [1] to describe the effective behavior of such composites in the macroscopic limit. The approach itself provides a very efficient calculation method for various situations and it is partially even analytically solvable. This allows a comprehensive understanding of the mechanisms underlying the behavior of magneto-sensitive elastomers and we are able to predict a discontinuous shape change for very oblate samples. It will also be shown, that the results for the case of a random isotropic distribution of magnetizable particles in the elastomer are in quantitative agreement with a micro-scale continuum model [2].

Literature
[1] *Romeis D. et. al.* Soft Matter **12**, 9364-9376 (2016)
[2] *Metsch P. et. al.* Comp. Mat. Science **124**, 365-374 (2016)

CPP 5.8 Mon 12:30 ZEU 255

Investigation of coated magnetic nanoparticles in polymer matrix via small-angle scattering methods — •Lisa Fruhner, Margarita Krutyeva, Wim Pyckhout-Hintzen, and Jürgen Allgaier — Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS-1) & Institute of Complex Systems (ICS-1), 52425 Jülich

Bringing magnetic nanoparticles into polymer matrices allows the creation of functional nanocomposites which offer a broad application range from sensors through electronics to smart coatings and human health. It is of great importance to be able to efficiently control the encapsulation and synthetic conditions regarding the minimization of agglomerates and creation of uniform hybrid nanomaterials

By making use of sophisticated synthesis techniques we obtain spherical nanoparticles in different size ranges with a small polydispersity. These nanoparticles are coated with a crosslinked shell consisting of the matrix polymer what allows them to be easily dispersed into the matrix and protects them against agglomeration.

Investigations via small-angle scattering methods and electron microscopy reveal the presence of mostly single nanoparticles and a small amount of linear chains consisting of a few particles. These systems are used as a basis for magneto-elastomeric nanocomposites with the structure controlled by mechanical or magnetic forces.

CPP 5.9 Mon 12:45 ZEU 255

Modeling bidisperse soft magnetic elastomers — •Pedro A. Sánchez[1], Sofia S. Kantorovich[1,2], Oleg V. Stolbov[3], and Yuriy L. Raikher[3] — [1]Computational Physics, University of Vienna, Sensengasse 8/18, 1090 Vienna, austria — [2]Ural Federal University, 3 Ural Federal University, Lenin av. 51, Ekaterinburg, 620000, Russia — [3]Institute of Continuous Media Mechanics, Ural Division of RAS, 1 Korolyov street, Perm, 614013, Russia

Soft magnetic elastomers are a type of hybrid materials consisting of a soft matrix of polymers in which a high volume fraction of magnetic micro- and/or nanoparticles are embedded. The elastic modulus of the polymer matrix is low enough to allow strong structural changes in the system induced by the response of the magnetic particles to external magnetic fields. These novel materials are promising candidates for a broad range of applications, like magnetically controlled dampers, magnetic field sensors, flow regulators or microfluidic pumps.

Here we present a bead-spring model of a soft magnetic elastomer material in which a combination of two types of magnetic particles are present within the polymer matrix: a low volume fraction of magnetically hard colloids—typically, ferromagnetic particles with diameters of 3-5 μm—and a high volumen fraction of weak magnetic particles—typically paramagnetic particles with a diameter of around 10nm. We analyze the magnetic response of this system by means of extensive computer simulations, and connect our results to analytical models based on continuum approaches.

CPP 6: Focus: Soft Particles in Flows I (joint focus session CPP/DY)

The dynamics and interactions of soft particles suspended in a flowing liquid are a physical problem of unusual complexity and of relevance in technical and biological systems, e.g. blood flow. The close connection between sophisticated numerical simulations and experiments has brought about a wealth of new insights in the recent past. The aim of the session is to review some of these recent advances, both experimental and theoretical/computational.

Organized by S. Gekle, G. Gompper, C. Wagner

Time: Monday 10:15–13:15 Location: ZEU 160

Invited Talk CPP 6.1 Mon 10:15 ZEU 160

Immersed Boundary Methods for Rigid and Deformable Particles in Viscoelastic flows — •Eric Shaqfeh — Department of Chemical Engineering, Stanford University

The immersed boundary method will be used with a finite volume fluid solver to develop a unique tool to examine the properties of a viscoelastic suspension of particles. The tool will employ unstructured grids and is massively parallel, thus allowing very complex geometries to be simulated. Since the internal stress of the particles is handled using a finite element solver, nearly arbitrary stress-strain relationships for the particles can be handled and their shape can deform continuously. A number of interesting physical problems will be examined with the code including 1) Sedimentation of particles in orthogonal shear and 2) the rheology of particulate suspensions in a viscoelastic fluid under shear.

CPP 6.2 Mon 10:45 ZEU 160

A new look at blood shear-thinning — Luca Lanotte[1], Johannes Mauer[2], Simon Mendez[3], Dmitry Fedosov[2], Jean-Marc Fromental[4], Viviana Claveria[1], Franck Nicoud[3], Gerhard Gompper[2], and •Manouk Abkarian[1] — [1]Centre de Biochimie Structurale, Montpellier, France — [2]Institute of Complex Systems and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany — [3]Institut Montpelliérain Alexander Grothendieck, Montpellier, France — [4]Laboratooire Charles Coulomb, Montpellier, France

Blood viscosity decreases with shear stress, a property essential for an efficient perfusion of the vascular tree. Shear-thinning is intimately related to the dynamics and mutual interactions of red blood cells (RBCs), the major component of blood. Because of the lack of knowledge about their behavior under physiological conditions, the link between RBCs dynamics and blood rheology remains still unsettled. Performing experiments and simulations in microcirculatory flow conditions of viscosity, shear rates and volume fractions, our work reveals how rich RBCs dynamic morphologies govern blood shear thinning, contrary to the current paradigm assuming steady RBC orientation and membrane circulation. Our results suggest that any pathological change in RBCs* local rheology will impact the onset of these morphological transitions and should play a key role in pathological blood flow.

CPP 6.3 Mon 11:00 ZEU 160

Clustering of microscopic particles in stenosed blood flow — •Christian Bächer, Lukas Schrack, and Stephan Gekle — Biofluid Simulation and Modeling, University of Bayreuth, Germany

A mixed suspension of red blood cells and microparticles flows through a cylindrical channel with a constriction mimicking a stenosed blood vessel. Our three-dimensional Lattice-Boltzmann simulations show that the red blood cells are depleted right ahead and after the constriction. For the red blood cells the axial concentration profile is very similar to that of isolated tracer particles flowing along the central axis. Most importantly, however, we find that the stiff microparticles exhibit the opposite behavior. Arriving on a marginated position near the channel wall, they can pass through the constriction only if they find a suitable gap to dip into the dense plug of red blood cells occupying the channel center. This leads to a prolonged dwell time and, as a consequence, to a pronounced increase in microparticle concentration right in front of the constriction. Similar clustering events occur for marginated particles in a cylindrical channel branching into two daughter channels.

CPP 6.4 Mon 11:15 ZEU 160

Margination of blood cells — •Revaz Chachanidze[1,2], Marc Leonetti[1], and Christian Wagner[2] — [1]Institut de Recherche sur les Phénomènes Hors Equilibre (I.R.P.H.E), Aix-Marseille University, Marseille, France — [2]Saarland University, Saarbruken, Germany

In blood flow erythrocytes migrate to the centre of the vessel creating a *cell-free layer* at the edge while leucocytes, lymphocytes and platelets tend to migrate to vessel walls. This phenomenon is known as margination. Margination of leucocytes and its role in immune response as well as margination of red blood cells in cases of some diseases (such as malaria and sickle cell disease) have been subjects of research for a while. Recent advances in targeted drug delivery arouses interest to margination of micro- and nano-particles.

Our research is dedicated to better understanding of mechanical properties of particles involved in margination and to create conditions for blood flow under which particles manifest tendency to segregation. For this purposes we observe and quantify blood flow consisting of 2 populations of red blood cells * healthy and rigidified with cross-linking agent (glutaraldehyde) * in microfluidic channels in cases of different volumetric flow rate, cells concentration and etc.

15min. break

Invited Talk CPP 6.5 Mon 11:45 ZEU 160

Effect of bending on the dynamics of a spherical capsule in shear flow — •Anne-Virginie Salsac — CNRS - Universite de Technologie de Compiegne, Compiegne, France

Encapsulating liquid droplets within a membrane enables to protect fragile or volatile substances and control their liberation. Typical artificial capsules are quasi*spherical at rest and present a hyperelastic membrane with mechanical and geometrical properties that are function of the fabrication process. When suspended in a simple shear flow, such capsules are elongated in the straining direction by the hydrodynamic stresses, while the membrane rotates around the deformed shape under the flow vorticity. But, for low flow strength, the capsule membrane is compressed in the equatorial region and blucking may occur. Since membrane wrinkling can cause fatigue breakup, it is important to predict it in order to avoid/provoke membrane rupture. The objective of the study is thus to study numerically an initially spherical capsule in shear flow and analyze the influence of the membrane bending rigidity on the capsule dynamics and wrinkle formation. The 3D fluid-structure interactions are modeled coupling a boundary integral method to solve for the internal and external Stokes flows with a thin shell finite element method to solve for the wall deformation [1]. For a given wall material, the capsule deformability strongly decreases when the wall thickness (or bending resistance) increases. We show that the global capsule motion and deformation can, however, be inferred from the ones obtained by a membrane model devoid of bending stiffness, as they are mainly governed by in-plane membrane tensions.

CPP 6.6 Mon 12:15 ZEU 160

Hydrodynamic mechanism of shear-induced ordering in weakly confined suspensions of deformable particles — •Alexander Farutin[1,2], Zaiyi Shen[1,2], Thomas Fischer[3], Jens Harting[4,5], and Chaouqi Misbah[1,2] — [1]Univ. Grenoble Alpes, LIPHY, F-38000 Grenoble, France — [2]CNRS, LIPHY, F-38000 Grenoble, France — [3]Laboratory for Red Cell Rheology, 52134 Herzogenrath, Germany — [4]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IEK-11), Forschungszentrum Jülich, Fürther Strasse 248, 90429, Nürnberg, Germany — [5]Department of Applied Physics, Eindhoven University of Technology, P.O. Box 513, 5600MB Eindhoven, The Netherlands

It has been shown recently by experiments and numerical simulations that suspensions of red blood cells confined between two walls can undergo ordering when subject to shear flow. In this presentation, we propose a hydrodynamical model that explains this effect. The key ingredients of the model are (1) wall-induced migration, which keeps the cells close to the midplane between the two walls, (2) long-range hydrodynamic interactions in the direction parallel to the walls, which cause cell pairs to align with the flow direction and to get attracted to each other and (3) short-range hydrodynamic interactions perpendicular to the walls, which cause the cells move out of the midplane in such a way that the shear flow pushes them apart. We have verified by solving our model analytically that two cells form a stable stationary pair. The intercell distance given by our model agrees with the experiments and the simulations.

CPP 6.7 Mon 12:30 ZEU 160

Ultrasound-triggered margination of microbubbles for targeted drug delivery — •Achim Guckenberger and Stephan Gekle — Biofluid Simulation and Modeling, Universität Bayreuth, Germany

During circulation through the vascular system, drug delivery agents should be preferably located in the low-shear interior of the blood stream. Yet, when they are close to the pathological region, they should attain a near-wall position for the most efficient interaction with the endothelium. Using mesoscopic three-dimensional numerical simulations we show that this apparent contradiction can be resolved by using phospholipid coated microbubbles. Application of an ultrasound pulse triggers the rapid migration of the microbubbles toward the endothelial walls due to the hydrodynamic interactions with the red blood cells. The effect is caused by the oscillations of the bubbles, resulting in alternations between a soft and a stiff state, as induced by the lipid shell. We find that the effect is very robust, being triggered even if the time spent in the stiff state is three times lower than the opposing time in the soft state.

CPP 6.8 Mon 12:45 ZEU 160

Inertial migration of elastic capsules in Poiseuille flow — •Christian Schaaf, Kevin Irmer, Christopher Prohm, and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany

Deformable particles such as capsules, vesicles and red blood cells assemble at fixed equilibrium positions in a microfluidic channel under Poiseuille flow. This behavior can be used to separate particles with different mechanical properties. For example, softer cancer cells travel closer to the center than healthy ones.

Using the Lattice-Boltzmann method, we study the dynamics of single deformable particles in a microfluidic channel for intermediate Reynolds numbers.

We show that particles move to different equilibrium position depending on their size and deformability. For Reynolds numbers below 100, their equilibrium positions collapse onto a single master curve depending only on the Laplace number. By applying external forces along the channel axis, we are able to control the equilibrium distance from the channel centerline and thereby have a means to enhance the sensitivity of particle separation.

CPP 6.9 Mon 13:00 ZEU 160

Migration reversal of soft particles in flows through wavy microchannels — •Matthias Laumann[1], Alexander Farutin[2], Chaouqi Misbah[2], Diego Kienle[1], and Walter Zimmermann[1] — [1]Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Laboratoire Interdisciplinaire de Physique, CNRS Universite Alpes, UMR 5588, BP 87, F-28402 Saint-Martin, d'Heres Cedex, FranceH

We study soft particles in low Reynolds number flows through microchannels with wavy boundaries. In low Reynolds number flows through microchannels with straight boundaries, soft particles often tend via cross-streamline migration to the channel center (see e.g. [1]). We show, that for wavy channel boundaries this centric motion may be reversed once the modulation amplitude exceeds a (parameter dependent) threshold, in which case the soft particles migrate to off-center trajectories. This is shown by semi-analytical and numerical results for flexible dumbbells, models for ring polymers and capsules in microflows. The distance between off-center trajectories and the center of the microchannel depends on the particle's elasticity and flow velocity as well as on the wavelength and the amplitude of the boundary modulation. Moreover, by increasing the flow velocity the migration direction may be reversed from out- to inward. Our insights can be exploited for particle separation with different properties in microchannels.

[1] B. Kaoui, G. H. Ristow, I. Cantat, C. Misbah, W. Zimmermann, Phys. Rev. E **77**, 021903 (2008).

CPP 7: Organic Electronics and Photovoltaics I: Light-Emitting Devices (joint session CPP/DS/HL, organized by CPP)

Time: Monday 11:00–13:00 Location: ZEU 260

CPP 7.1 Mon 11:00 ZEU 260

Two-color warm white hybrid OLEDs from thermally activated delayed fluorescence — •Ludwig Popp[1], Paul Kleine[1], Reinhard Scholz[1], Ramunas Lygaitis[1,2], Olaf Zeika[1], Axel Fischer[1], Simone Lenk[1], and Sebastian Reineke[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, TU Dresden, Germany — [2]Kaunas University of Technology, Lithuania

Thermally activated delayed fluorescence (TADF) takes place in organic molecules where the energy splitting between the lowest excited singlet and triplet states (ST-splitting, ΔE_{ST}) remains sufficiently low. A newly designed sky-blue TADF emitter with an emission maximum at a wavelength of 500 nm reaches a photoluminescence quantum yield of 70% and an external quantum efficiency (EQE) of up to 14.5% in actual organic light-emitting devices (OLEDs).

In this work we use the sky-blue TADF molecule to build warm white hybrid OLEDs by combination with the red phosphorescent emitter Ir(MDQ)$_2$(acac). Due to the very broad TADF emission, covering a majority of the high-energy visible spectrum, a dedicated deep blue emitter is becoming obsolete for reaching high color rendering indices (CRI $>$ 80).

Furthermore, we demonstrate deeper insight into the energy transfer mechanisms in this hybrid TADF/phosphorescence approach. Time-correlated single photon counting enables to determine the actual exciton decay pathways and delivers a detailed understanding of the excitonic interplay between the particular excited states.

CPP 7.2 Mon 11:15 ZEU 260

Conjugation induced thermally activated delayed fluorescence — •Paul Kleine[1], Qiang Wei[2], Yevhen Karpov[2], Xianping Qiu[2], Hartmut Komber[2], Karin Sahre[2], Anton Kiriy[2], Ramunas Lygaitis[1], Simone Lenk[1], Brigitte Voit[2], and Sebastian Reineke[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Dresden, Germany — [2]Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany

Thermally activated delayed fluorescence (TADF) has seen tremendous research efforts in the last years. It represents an alternative to phosphorescent emitter materials in organic light-emitting diodes, assuring 100% internal quantum efficiency via effective reverse intersystem crossing of barely radiative triplet to emissive singlet states. While many small molecules have been reported to show efficient TADF, reports on polymers sporting TADF are rare. Up to now, publications cover concepts only, where TADF chromophores are linked to polymer networks, retaining their monomeric properties. In this talk, we discuss a novel strategy that unlocks an additional molecular design rule reserved exclusively for polymeric materials. A π-conjugated cyclic polymer composed of non-TADF building blocks was developed. Conjugation induced HOMO destabilization leads to a decreased singlet-triplet splitting and efficient TADF in the polymer, while the repeating unit shows only inefficient phosphorescence. This conjugation induced TADF concept represents a novel molecular design rule particularly for solution-processable polymeric materials.

CPP 7.3 Mon 11:30 ZEU 260

Investigation of organic light emitting diodes based on thermally activated delayed fluorescence via magnetic resonance methods — •Nikolai Bunzmann[1], Sebastian Weissenseel[1], Benjamin Krugmann[1], Jeannine Grüne[1], Stefan Väth[1], Andreas Sperlich[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Organic light emitting diodes (OLEDs) based on thermally activated delayed fluorescence (TADF) exhibit a high upconversion rate from non-emissive triplet to emissive singlet states due to a small energy splitting ΔE_{ST} between the respective states. Consequently, the internal quantum efficiency (IQE) of such devices is strongly enhanced. However, the underlying mechanism of reverse intersystem crossing (RISC) is naturally spin forbidden, wherefore spin sensitive measurement methods are desirable in order to elucidate the TADF process. Therefore, we use electrically and electroluminescence detected magnetic resonance (EDMR, ELDMR) techniques. Hereby, transitions between triplet substates, which are split in an external magnetic field, are driven by microwaves, applied via a non-resonant stripline. We evaluate the dependence of multi-frequency ELDMR and EDMR spectra on changes in experimental conditions in order to obtain detailed information about the investigated spin system. Thereby we contribute to a better understanding of the TADF mechnism, which is crucial in order to further improve the performance of OLED based light sources.

CPP 7.4 Mon 11:45 ZEU 260

Orientation of Phosphorescent Dopants in Organic Vapor Phase Deposited Films — •Thomas Lampe[1], Matthew J. Jurow[3], Francisco F. Navarro[2], John Facendola[2], Tobias D. Schmidt[1], Peter I. Djurovich[2], Mark E. Thompson Thompson[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Department of Chemistry, University of Southern California, Los Angeles, California 90089, United States — [3]The Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States

Organic vapor phase deposition (OVPD) is an efficient film deposition technique for the preparation of organic thin films. However, the atmospheric conditions during deposition differ from the common thermal evaporation in high vacuum. To investigate the effects of these differences on heteroleptic phosphor orientation in organic guest-host systems we deposited films via OVPD while controlling the substrate temperature during deposition. The measurement of the alignment of the emissive transition dipole moments in samples deposited at room temperature leads to results comparable to preparation via thermal evaporation. Deposition of the film on a cooled substrate reveals a thermally activated behaviour of the molecular alignment process at low temperatures. The confirm an earlier model for the molecular alignment of heteroleptic phosphopors and give further insight into the physical properties of this phenomenon.

[1] M. Jurow, et. al.: *Nature Mat.* **15** (2015), 85-91

CPP 7.5 Mon 12:00 ZEU 260

Magnetic resonance at ultra-small fields in PPV-based OLEDs — •Hermann Kraus, Viola Zeller, Sebastian Bange, and John M. Lupton — Universität Regensburg, Universitätsstraße 31, 93053 Regensburg, Deutschland

Large magnetoresistance and magnetoluminescence effects which arise, for example, due to spin-dependent recombination rates are well-known for OLEDs, although models are still under debate given that they remain hard to verify from a measurement of integrated current and luminance. At very low fields a change in the sign of magnetoresistance appears: the so called ultra-small magnetic field effect for which also several models exist.

Spin resonance of paramagnetic species enables direct manipulation of charge carrier and excitonic precursor spins but most work on spin resonance in OLEDs was done at external magnetic fields on the order of several hundred millitesla. While it is also possible to perform these experiments at fields down to a few millitesla it was believed that resonance effects disappear once the external field is of the same order of magnitude as the internal hyperfine fields. We show that electron spin resonance signals are detectable through both the current and the electroluminescence at ultra-small fields corresponding to a few MHz resonance frequency. This demonstration provides insights into the ultra-small magnetic field effect in magnetoresistance as well as testing the principles of magnetic resonance for very low Zeeman splitting.

CPP 7.6 Mon 12:15 ZEU 260

Ultrathin metal electrode for bottom-emitting OLEDs on buckled substrates — •Yungui Li, Toni Bärschneider, Paul-Anton Will, Yuan Liu, Simone Lenk, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonics Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, 01062 Dresden, Germany

We here report our investigations on nanometer thick, composite ultrathin metal electrodes used in organic light-emitting diodes (OLEDs) comprising buckled substrates. The thin metal electrodes are made of 1 nm molybdenum trioxide (MoO3), 2 nm gold, and 3-15 nm of silver. A composite electrode with 9 nm silver based on flat glass substrate shows a maximum transparency of about 80% at 455 nm and a sheet resistance of 10 Ω/sq. With reactive-ion etching process, a buckled surface with depths around 50 to 100 nm is designed to extract the trapped light of bottom-emitting OLEDs since total internal reflection in flat device. When the thin metal electrode is utilized for green bottom-emitting OLEDs, the devices show a maximum external quantum efficiency of 17.5% for buckled OLEDs while in contrast only 13.8% for flat devices. Compared to flat devices, buckled devices show the same level of leakage current and better color stability at different angles. The results confirm the high potential of composite thin metal systems as alternative electrode for OLEDs, with the capability of application for bottom- and top-emitting OLEDs on patterned surfaces.

CPP 7.7 Mon 12:30 ZEU 260

Impact of charge carrier injection on single-chain photophysics of conjugated polymers — •Felix J. Hofmann, Jan Vogelsang, and John M. Lupton — Universität Regensburg

Charges in conjugated polymer materials have a strong impact on the photophysics and their interaction with the primary excited state species has to be taken into account in understanding device properties. Here, we employ single-molecule spectroscopy to unravel the influence of charges on several photoluminescence (PL) observables. The charges are injected either stochastically by a photochemical process, or deterministically in a hole-injection sandwich device configuration. We find that upon charge injection, besides a blue-shift of the PL emission and a shortening of the PL lifetime due to quenching and blocking of the lowest-energy chromophores, the non-classical photon arrival time distribution of the multichromophoric chain is modified towards a more classical distribution. Surprisingly, the fidelity of photon antibunching deteriorates upon charging, whereas one would actually expect the number of chromophores to be reduced. A qualitative model is presented to explain the observed PL changes. The results are of interest to developing a microscopic understanding of the intrinsic charge-exciton quenching interaction in devices.

CPP 7.8 Mon 12:45 ZEU 260

Optical Detection of the Magnetic Field Effect in OLEDs with Metal-Free Dual Singlet-Triplet Emitters — •Wolfram Ratzke[1], Lisa Schmitt[2], Hideto Matsuoka[2], Christoph Bannwarth[2], Marius Retegan[3], Jonas Zipfel[1], Sebastian Bange[1], Philippe Klemm[1], Frank Neese[3], Stefan Grimme[2], Olav Schiemann[2], John Lupton[1], and Sigurd Höger[2] — [1]University of Regensburg, Germany — [2]University of Bonn, Germany — [3]MPI Mühlheim an der Ruhr, Germany

Even though the magnetic field effect of organic light emitting diodes (OLEDs) has been investigated for more than one decade it is still difficult to identify the underlying mechanisms. Furthermore, theories are discussed which are based on the magnetic field dependent formation of singlet and triplet excited states in order to explain the change in the device resistance without a simultaneous experimental access to all three observables. The spin states can be measured by detecting the fluorescence and phosphorescence but so far this was always restricted to the exclusive observation of pure singlet or triplet emission by investigating different molecular systems, and hence a coherent statement is not possible. Recently, we have developed metal-free OLED emitters which exhibit simultaneous fluorescence and phosphorescence, even at room temperature. These materials can give insight into the change of spin-state statistics when an external magnetic field is applied, and offer a new perspective to distinguish between different field regimes and spin-dependent mechanisms which lead to the magnetic field effect.

CPP 8: Fundamentals of Perovskite Photovoltaics II (joint session CPP/DS/HL)

Time: Monday 15:00–18:15 Location: ZEU 222

Invited Talk CPP 8.1 Mon 15:00 ZEU 222

Visualizing Charge Carrier Diffusion In Hybrid Halide Perovskite Thin Films — •Achim Hartschuh, Kathrin Handloser, Irene Grill, Nicolai Hartmann, Nadja Giesbrecht, Meltem Aygüler, Mathhias Handloser, Thomas Bein, and Pablo Docampo — Department of Chemistry and CeNS, LMU Munich, 81377 Munich, Germany

Organic-inorganic metal halide perovskites represent one of the most promising classes of absorber materials for future photovoltaic applications [1]. A prerequisite for the efficient extraction of photo-generated carriers is the combination of low non-radiative relaxation rates and rapid diffusive transport. We study the excited state dynamics and charge carrier transport properties in different perovskite thin films using time-resolved photoluminescence microscopy. By scanning the confocal detection with respect to the excitation spot, we visualize diffusive transport on micrometer length scales and determine the charge carrier diffusion constants and mobilities [2]. We complement these studies by transient photocurrent measurements on the same films and derived devices [3,4].

Invited Talk CPP 8.2 Mon 15:30 ZEU 222

Photon recycling in hybrid lead-halide perovskite semiconductors — •Felix Deschler — University of Cambridge, Cambridge, UK

We discuss the effect of photon recycling on the externally measured radiative recombination rates in hybrid perovskites. By combining transient absorption with transient photoluminescence (PL) data, we distinguish radiative from non-radiative processes and find that the PL originates from a bimolecular process for all investigated carrier densities. We measure external photoluminescence quantum efficiencies (PLQEs) under continuous-wave and pulsed excitation. Taking into account photon recycling, we connect the externally measured radiative efficiencies with the actual internal values, and derive internal PLQEs exceeding 80%.

We map the propagation of photo-generated luminescence and charges from a local photo-excitation spot in thin films of lead triiodide perovskites using a confocal microscopy setup. We observed regenerated PL emission at distances as far as 50 micrometers away from photo-excitation. We map the internal photon distribution in the film and find that, over these distances, the peak of the internal photon spectrum red-shifts from 765 to >800 nanometers. We build a lateral-contact solar cell with selective electron- and hole-collecting contacts, using a combination of photo-lithography and electro-deposition. We used these devices as a platform to study photocurrent propagation and found that charge extraction can be achieved well beyond 50 micrometers away from the excitation.

CPP 8.3 Mon 16:00 ZEU 222

Coherent Dynamics of Free Exciton Dissociation in Lead-iodide Perovskites observed by 2D Electronic Spectroscopy — •Ajay Jha[1], Hong-Guang Duan[1,2,3], Vandana Tiwari[1], Pabitra Nayak[4], Michael Thorwart[2,3], Henry J. Snaith[4], and R. J. Dwayne Miller[1,3,5] — [1]MPI-Structure & Dynamics of Matter, Hamburg, Germany — [2]Universität Hamburg,Germany — [3]CUI Hamburg, Germany — [4]University of Oxford, UK — [5]University of Toronto, Canada

Hybrid organolead halide perovskites with high carrier mobility and large dielectric constant have received considerable attention as an excellent material for low-cost efficient photovoltaics. The power conversion efficiency of perovskite based solar cells has meteorically advanced to 22.1% with excitonic dye-sensitization concept and ~15% for planar heterojunction configuration. The unprecedented success of this material demands the fundamental understanding of underlying microscopic mechanisms for photoinduced charge generation. Recent studies suggest that most photoexcitations in perovskite are free charge carriers behaving like III-V inorganic semiconductors, but the contribution of excitons has been a matter of debate. We have employed ultrafast 2D electronic spectroscopy to probe elementary optical excitation of CH3NH3PbI3 thin films. We distinctly observe the electronically coupled excitonic and free carrier transitions at room temperature. We captured an ultrafast exciton dissociation favored by low exciton binding energy of ~40 meV. The interplay of strongly coupled dominant vibrational mode to exciton dynamics will also be discussed.

CPP 8.4 Mon 16:15 ZEU 222

Time Resolved Microwave Conductivity on Perovskites — •Marvin Grüne[1], Andreas Sperlich[1], Andreas Baumann[2], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

Organo-metal halide perovskites continue to be the star of thin film solar cells exhibiting rapidly rising power conversion efficiencies. For further improvement of these solar cells it is essential to understand the fundamental intrinsic properties like photoconductivity, recombination and charge carrier mobility. Therefore, we investigate the mixed halide perovskite layers of $CH_3NH_3PbX_3$ (X: I^-, Br^- and Cl^-) using time-resolved microwave conductivity. With this contactless measurement technique we address the charge carrier lifetime, decay kinetics and intrinsic mobility of perovskite structures with different halide substituents X. The mobility increases more than a factor of 2 in this order of substituents up to 8 cm^2/Vs. Furthermore, the influence of solvent annealing on the crystallization process of the $CH_3NH_3PbI_3$ film has been investigated, now considering temperature dependence. This crystallization method generates e.g. bigger crystal domain sizes and almost one order of magnitude higher mobilities. Due to the absence of transport layers, we can relate differences in the results to intrinsic properties of the perovskite layers. Solar cells with the investigated layer achieve up to 16% efficiency in our labs.

15 min break

Invited Talk CPP 8.5 Mon 16:45 ZEU 222

Interface engineering: the route towards high efficiency and stable hybrid perovskite solar cells — •Giulia Grancini — Group for Molecular Engineering of Functional Materials, EPFL Valais Wallis, CH-1951 Sion, Switzerland

Hybrid perovskite solar cells are undoubtedly leading the photovoltaic scene with their power conversion efficiency (PCE) >22%. Tuning the material composition, i.e. by cations and anions substitution (e.g. introducing a small amount of Br) and the interfacial properties, optimizing the structural and chemical interactions and the optoelectronic processes therein have been the successful routes for a real breakthrough in device efficiency and reproducibility. However, despite the impressive PCE reported, hybrid perovskite suffer of severe instability mainly due to material degradation upon exposure to water and moisture further accelerated under local heating and UV irradiation. Diverse technological approaches have been proposed delivering appreciable improvements, but still failing by far the market requirements. Recently, we pioneered a new concept by interface engineering a multi-dimensional composite of two dimensional (2D) (HOOC(CH2)2NH3)2PbI4 / 3D-CH3NH3PbI3 perovskite molecular junction. The composite forms an exceptional gradually organized structure that yields up to 12.9% PCE. Aiming at the up-scaling of this technology, we realize 10x10 cm2 large-area solar modules by a fully printable, industrial-scale process delivering 11.2% stable devices for 9,000 hours under accelerated testing conditions, leading to a record one-year stability.

CPP 8.6 Mon 17:15 ZEU 222

Characterization of perovskite solar cells: Towards a reliable measurement protocol — •Eugen Zimmermann[1], Ka Kan Wong[1], Michael Müller[1], Hao Hu[1], Philipp Ehrenreich[1], Markus Kohlstädt[2,3], Uli Würfel[2,3], Simone Mastroianni[2], Gayathri Mathiazhagan[2], Andreas Hinsch[2], Tanaji P. Gujar[4], Mukundan Thelakkat[4], Thomas Pfadler[1], and Lukas Schmidt-Mende[1] — [1]Universität Konstanz, Konstanz, Germany — [2]Fraunhofer Institute for Solar Energy Systems ISE, Freiburg, Germany — [3]Freiburg Materials Research Center FMF, University of Freiburg, Freiburg, Germany — [4]Applied Functional Polymers, Department of Macromolecular Chemistry I, University of Bayreuth, Bayreuth, Germany

Tremendous progress on power conversion efficiency of lead halide perovskite solar cells during the last few years drastically increased the interest in research on this material. However, a so called "hysteretic" behaviour during current density-voltage (J-V) measurements is differently severe for differently prepared solar cells and strongly depends on scan parameters like scan rate, and measurement history. This challenges reliable results across different laboratories and hinders the aspect of commercialization. Here, we propose a reliable measurement protocol by introducing stabilized device characteristics obtained from an adaptive tracking of the maximum power point and the open circuit voltage, and compare such obtained values to device characteristics derived from standard and time resolved J-V measurements for varying solar cells fabricated in different laboratories.

CPP 8.7 Mon 17:30 ZEU 222

Removing leakage recombination current in planar perovskite solar cells — •Kristofer Tvingstedt[1], Lidon Gil-Escrig[2], Christina Momblona[2], Philipp Rieder[1], David Kiermasch[1], Andreas Baumann[3], Henk J. Bolink[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximillian University of Würzburg, 97074 Würzburg — [2]Instituto de Ciencia Molecular, Universidad de Valencia, C/Catedrático J. Beltrán 2, 46980 Paterna, Spain — [3]Bavarian Center for Applied Energy Research 97074 Würzburg

All solar cells, including perovskites, suffer from recombination mechanisms of various types out of which leakage current usually dominates at lower voltages. Herein, we demonstrate a three order reduction of this recombination loss mechanism in planar perovskite solar cells by replacing the commonly used hole selective electrode PEDOT:PSS with a polymer arylamine hole transporting semiconductor. This renders these solar cells more useful under lower light intensity, such as end of the day and indoor conditions which we demonstrate via the extreme case of moon lighting conditions, where the cells still generates open circuit voltages of 530 mV. By this substantial leakage reduction we can be able to confirm charges to also remain in the photovoltaic device for up to 2 hours after the light has been switched off. We discuss the mechanisms behind this feature and explain why the arylamine is a superior hole selective electrode.

CPP 8.8 Mon 17:45 ZEU 222

Double-layer charge selective contacts in perovskite solar cells as a key to improved efficiency and reduced hysteresis effects — •Lukas Kegelmann[1], Christian Wolff[3], Celline Awino Omondi[1], Lars Korte[1], Thomas Dittrich[1], Dieter Neher[3], Bernd Rech[1], and Steve Albrecht[2] — [1]Helmholtz-Zentrum Berlin, Inst. for Silicon Photovoltaics, Berlin, 12489, Germany. — [2]Helmholtz-Zentrum Berlin, Young Investigator Group Perovskite Tandem Solar Cells, Berlin, 12489, Germany. — [3]University of Potsdam, Soft Matter Physics, Potsdam, 14476, Germany.

Planar low-temperature processed perovskite solar cells without a mesoscopic scaffold are advantageous for a possible large-scale production but often suffer from photocurrent hysteresis, especially in the regular 'n-i-p'-structure. Here, we systematically study the influence of different low-temperature deposited electron transport materials (ETM) on planar regular solar cell characteristics. We further show that an elaborately chosen metal oxide interlayer in an ITO/metal oxide/PCBM double-layer ETM can significantly improve the device performance. J-V measurements reveal substantial reductions of hysteresis effects and enhanced power conversion efficiencies up to a champion stabilized value of 18.0 % for TiO2 interlayers. Surface photovoltage spectroscopy is used to show comparable absorber qualities on all ETMs for the fabrication process used here. Additionally, improved hole blocking for the double-layer structure is suggested by UPS and the metal oxide interlayer is considered to reduce shunt paths as it hampers direct contact between perovskite and the ITO electrode.

CPP 8.9 Mon 18:00 ZEU 222

Electrical impedance spectroscopy on perovskite solar cells — •Fischer Mathias[1], David Kiermasch[1], Vladimir Dyakonov[1,2], and Andreas Baumann[2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research, 97074 Würzburg

Electrical impedance spectroscopy has shown to be a powerful technique to obtain informations about key parameters of a solar cell, like series and recombination resistance, build-in potential and the dielectric constant. Here, we performed impedance measurements over a wide temperature range from 300K down to 150K on solution processed CH$_3$NH$_3$PbI$_3$ perovskite solar cells. We compared the impedance spectra of n-i-p and p-i-n device configuration which is FTO/TiO$_2$/Perovskite/Spiro-MeOTAD/Au and ITO/PEDOT:PSS/Perovskite/PC$_{60}$BM/C$_{60}$/BCP/Au, respectively. We fit the impedance spectra by using corresponding equivalent circuits to investigate the dielectric behavior depending on the cell layout and preparation technique. We compare the extracted time constants at different frequency domains to reveal the influence from the p- and n-layer materials on the photovoltaic properties of the perovskite absorber material itself and examined charge carrier recombination behavior in dependency of illumination intensity.

CPP 9: Organic Electronics and Photovoltaics II: Doping (joint session CPP/DS/HL, organized by CPP)

Time: Monday 15:00–18:15 Location: ZEU 260

Invited Talk CPP 9.1 Mon 15:00 ZEU 260

Molecular Electrical Doping of Organic Semiconductors — •Ingo Salzmann — Humboldt Universität zu Berlin, Berlin, Germany

In contrast to inorganic semiconductors, the potential of doping organic semiconductors (OSCs) for enabling new functionality and improving opto-electronic device performance has only recently been established. Here, the broad range of phenomena observed upon molecularly doping conjugated polymers (CPs) and molecules (COMs) is discussed, from which, finally, two different competing scenarios emerge [1]: (i) the formation of both OSC and dopant ions through integer-charge transfer, i.e., an ion pair (IPA), and (ii), the emergence of OSC/dopant ground-state charge transfer complexes (CPXs). In particular, the doping of poly(3-hexylthiophene) (P3HT) will be juxtaposed with that of quaterthiophene (4T) where, for both systems, an increase in thin-film conductivity by several orders of magnitude is observed. The underlying doping mechanisms at work are, however, fundamentally different [2]: IPA formation occurs for the polymer while CPX formation is found for the chemically and structurally similar oligomer. For both cases (i) and (ii), the doping-induced modification of the OSC density of states (DOS) is generally discussed for both p- and n-doping and its Fermi-Dirac occupation is modelled by numerical simulations. Therefrom finally emerges that engineering the DOS of doped OSCs, the occupation of which ultimately determines the doping efficiency, represents a key challenge in dopant design.

[1] I. Salzmann et al., Acc. Chem. Res. 49, 370 (2016)

[2] H. Méndez et al., Nature Commun. 6, 8560 (2015)

CPP 9.2 Mon 15:30 ZEU 260

Inter-facial charge transfer studied in organic hetero-structure field-effect transistors. — •Eduard Meister, Stefan Schmidt, and Wolfgang Brütting — Institut für Physik, Universität Augsburg, Germany

In this work we studied inter-facial morphology dependent charge transfer (CT) happening in hetero-structure FETs based on vapour deposited small molecules. Therefore we used alpha-sexithiophene (α-6T) as donor and hexafluorotetracyanonaphthoquinodimethane (F$_6$TCNNQ) as acceptor. The lowest unoccupied molecular orbital of F$_6$TCNNQ is placed below of the highest occupied molecular orbital of α-6T, so that from an energetic point of view CT from α-6T to F$_6$TCNNQ molecules should occur. As evidence of CT we observed strong reduction of the switch-on voltage.

In order to get more information about morphology dependent CT and charge transport we produced devices with different gate insulator surfaces acting as template: blank SiO$_2$, as well as additional PMMA and thermally smoothed tetratetracontane [1] passivation layers. The morphology of α-6T layers was studied by atomic force microscopy and X-ray diffraction measurements. We employed also morphology dependent contact doping by application of tetrathiafulvalene tetracyanoquinodimethane salt contacts in contrast to mostly used gold electrodes. For the study of the transport mechanisms we performed temperature dependent measurements and calculated an upper limit of the activation energy for all the used configurations.

[1] L. Pithan et al., *J. Chem. Phys.* **143** (2015) 164707.

CPP 9.3 Mon 15:45 ZEU 260

Frontier orbital energy levels and exciton binding energies in organic charge transfer complexes — •Paul Beyer[1], Stefan Krause[2], Timo Florian[1], Eduard Meister[3], Lutz Grubert[4], Wolfgang Brütting[3], Norbert Koch[1,2], and Andreas Opitz[1] — [1]Dep. of Physics, Humboldt-Universität zu Berlin — [2]Helmholtz-Zentrum Berlin — [3]Institute of Physics, University of Augsburg — [4]Dep. of Chemistry, Humboldt-Universität zu Berlin

The frontier π-orbitals of planar molecules tend to overlap upon contact and hybridization takes place resulting in charge transfer complexes (CTC) with modified energy levels [1]. We characterize the energy levels for the materials diindenoperylene (DIP) and hexafluorotetracyanonaphthoquinodimethane (F6TCNNQ) in solution by cyclic voltammetry as well as in thin films and in planar heterojunction geometry by photoelectron spectroscopy. Optical transitions were measured by UV/Vis/NIR absorption and X-ray transitions by near edge X-ray absorption fine structure spectroscopy.

At the planar DIP/F6TCNNQ interface CTC formation occurs. Due to the energy level alignment at the interface, which will be shown in detail for standing and lying molecular orientations, and the lower gap of the CTC in contrast to the semiconductor DIP, doping is present and DIP field-effect transistors with F6TCNNQ deposited on top are showing a strongly reduced threshold voltage. Furthermore, the exciton binding energies, which are much larger for X-ray than for optical excitations, will be discussed together with the energy levels.

[1] H. Méndez et al., *Nat. Commun.* **6** (2015) 8560.

CPP 9.4 Mon 16:00 ZEU 260

Conical Intersection Dynamics of F4TCNQ Anion Radical doped Conducting Polymer Observed by 2D Electronic Spectroscopy — Ajay Jha[1], Hong-Guang Duan[1,2,3], •Vandana Tiwari[1], Michael Thorwart[2,3], and R. J. Dwayne Miller[1,3,4] — [1]MPI-Structure & Dynamics of Matter, Hamburg, Germany — [2]Universität Hamburg, Germany — [3]CUI Hamburg, Germany — [4]University of Toronto, Canada

Quinones are well celebrated electron acceptors which are even employed by nature for their impressive ability to retain electrons e.g. ubiquinone and plastoquinone. Quinone derivatives like tetrafluorotetracyano-quinodimethane (F4TCNQ) are popularly used as a p-type dopant to obtain high conducting polymer blend. To achieve higher conductivity, there has been a constant empirical effort to obtain different derivatives of quinones. In order to develop a molecular basis for rational tailoring F4TCNQ unit, understanding the electronic structure and relaxation dynamics of the TCNQ doped within a polymer framework is paramount. We have employed two-dimensional electronic spectroscopy to probe the coherent dynamics of F4TCNQ with the semiconducting polymer forming a charge transfer complex. We captured an ultrafast decay of F4TCNQ- mediated by conical intersection which is in agreement with the photoelectron spectroscopic studies in gas-phase. Additionally, we also observe that electronic transitions in F4TCNQ- are strongly coupled to polymer cation electronic structure. Our results open up new perspectives for tailoring intermolecular interactions to obtain high electrical conductivities.

CPP 9.5 Mon 16:15 ZEU 260

Electronic structure of charge transfer compounds using Fermi- Löwdin orbital self-interaction corrected DFT — •Torsten Hahn^1, Martin Knupfer^2, and Florian Rückerl^2 — ^{1}Institute for Theoretical Physics, TU Freiberg, Freiberg, Germany — ^{2}Institute for Solid State Research, IFW Dresden, Germany

We present experimental and theoretical results on novel Picene/F4TCNQ and related donor / acceptor systems [1,2]. The recently developed Fermi-Löwdin orbital based approach for self-interaction corrected density functional theory (FLO-SIC DFT [3,4]) is used to investigate the electronic structure of these materials. The theoretical results are compared to standard DFT calculations and experimental data obtained by photoemission spectroscopy. We focus our analysis on the description of the magnitude of the ground state charge transfer and on the details of the formed hybrid orbitals. Further, we show that for weakly bound donor / acceptor systems the FLO-SIC approach delivers a more realistic description of the electronic structure compared to standard DFT approaches.

[1] B. Mahns, et al., Cryst. Growth Des. 14, 1338 (2014).
[2] F. Rückerl et al., JCP 145, (2016).
[3] M. R. Pederson et al., JCP 140, 121103 (2014).
[4] M. R. Pederson, JCP 142, 064112 (2015).

15 min break

CPP 9.6 Mon 16:45 ZEU 260

UV-Vis-NIR spectroscopy studies on molecularly doped semiconducting polymers — •Malavika Arvind^1, Patrick Pingel^2, Silvia Janietz^2, and Dieter Neher^1 — ^{1}University of Potsdam, Soft Matter Physics, Germany — ^{2}Fraunhofer Institute for Applied Polymer Research, Potsdam, Germany

In recent years, significant efforts have been devoted towards understanding the fundamental processes involved in the doping of organic semiconductors with small molecules. Nevertheless, there is still a large degree of ambiguity in the field, which has prevented us from being able to truly exploit this method to better our organic devices. In this work, we utilize UV-Vis-NIR spectroscopy to study the sub-band gap optical transitions that occur in the well known semiconducting polymer poly(3-hexylthiophene) (P3HT) when doped with tris(pentafluorophenyl)borane (BCF), a strong Lewis acid, and compare it to the more commonly studied p-dopant, tetrafluorotetracyanoquinodimethane (F4TCNQ). In spite of the dissimilarity in their structures, both dopants are found to efficiently create positive polarons in P3HT, in solutions as well as in films. Here we investigate the influence of various parameters such as polymer/dopant concentration, solvent, temperature on the nature and efficiency of molecular doping, and also address the question of whether pre-aggregation of the polymer in solution assists or suppresses polaron-formation in P3HT.

CPP 9.7 Mon 17:00 ZEU 260

Redox-Potentials Outperform Ionization Energy / Electron Affinity for Predicting Ion Pair Formation in Molecular Electrical Doping — •Berthold Wegner^1, Lutz Grubert^2, Dennis Chercka^3, Andreas Opitz^4, Stefan Hecht^2, Klaus Müllen^3, and Norbert Koch^{1,4} — ^{1}Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — ^{2}Institut für Chemie, Humboldt-Universität zu Berlin, Berlin, Germany — ^{3}Max-Planck-Institut für Polymerforschung, Mainz, Germany — ^{4}Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

Electrical doping with strong molecular donors and acceptors is a key technological component to control the charge carrier density and Fermi level of organic semiconductors. While commonly ionization energy / electron affinity values (measured on thin films via ultraviolet / inverse photoelectron spectroscopy) are employed to guide the selection of molecular dopants for organic hosts, we find strong indications that redox-potentials (measured in solution via cyclic voltammetry) are indeed better suited. A set of donor-acceptor systems, both in solution and in thin films, is studied using structurally similar molecules. Our results show that redox-potentials provide a useful basis to predict ion pair formation in the studied systems, while ionization energies / electron affinities fail to provide such a basis. This is ascribed to the molecular length scale dopant-host interaction well described by local redox events at the molecule-electrode interface, whereas thin film ionization and affinity level measurements include collective and long-range solid state properties.

CPP 9.8 Mon 17:15 ZEU 260

Effective work function reduction of practical electrodes using an organometallic dimer — Kouki Akaike^1, Marco V. Nardi^1, Martin Oehzelt^{2,1}, Johannes Frisch^{2,1}, •Andreas Opitz^1, Christos Christodoulou^1, Giovanni Ligorio^1, Paul Beyer^1, Melanie Timpel^1, Igor Pis^3, Federica Bondino^4, Karttikay Moudgil^5, Stephen Barlow^5, Seth R. Marder^5, and Norbert Koch^{1,2} — ^{1}Humboldt-Universität zu Berlin, Germany — ^{2}Helmholtz-Zentrum Berlin, Germany — ^{3}Elettra-Sincrotrone Trieste, Italy — ^{4}IOM CNR Laboratorio TASC, Italy — ^{5}Georgia Institute of Technology, USA

The control of the cathode work function (WF) is essential to enable efficient electron injection and extraction at organic semiconductor/cathode interfaces in organic electronic devices. Here, ultraviolet photoelectron spectroscopy is used to determine the work function reduction by moderately air-stable pentamethylrhodocene dimer onto various conducting electrodes, by either vacuum deposition or drop casting from solution, to less than 3.6 eV, with 2.7 eV being the lowest attainable value. Electron transfer from the molecule to the respective substrates is responsible for the appreciable WF reduction. Notably, even after air exposure, the WF of the donor-covered electrodes remains below those of typically used clean cathode metals, such as Al and Ag. This demonstrates the ability of the pentamethylrhodocene dimer to reduce the WF for a wide range of electrodes used in all-organic or organic-inorganic hybrid devices.

K. Akaike et al., *Adv. Funct. Mater.* **26** (2016) 2493-2502.

CPP 9.9 Mon 17:30 ZEU 260

Temperature-induced F4TCNQ desorption from p-doped P3HT films — •Hannes Hase^1, Andreas Opitz^1, Norbert Koch^{1,2,3}, and Ingo Salzmann^1 — ^{1}Humboldt-Universität zu Berlin, Supramolekulare Systeme, Germany — ^{2}Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Bereich Solarenergieforschung, Germany — ^{3}Jiangsu Key Laboratory for Carbon-Based Functional Materials & Devices, Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou 215123, P.R. China

Thermal post-fabrication annealing is common practice for functional conjugated polymer (CP) films in organic photovoltaic cells, which is also applied to p-doped CPs in a number of studies. However, the typically small molecular-weight dopants, like, e.g., tetrafluorotetracyanoquinodimethane (F4TCNQ), can be expected to be prone to diffusion upon thermal treatment, which has been largely disregarded in pertinent literature. Here, we explore to which extent the annealing temperature impacts films of poly(3-hexylthiophene-2,5-diyl) (P3HT) doped with F4TCNQ. For temperatures beyond 60 °C, we find a reduction in conductivity with a concomitantly lowered dopant concentration, as deduced from optical and Fourier-transform infrared spectroscopy. While atomic force microscopy indicates the morphology to be essentially retained, grazing-incidence X-ray diffraction confirms the transition from a P3HT/F4TCNQ mixed crystal structure to pure P3HT and points towards F4TCNQ desorption. We conclude that, upon thermal annealing, dopant loss needs to be accounted for by adjusting the dopant concentration.

CPP 9.10 Mon 17:45 ZEU 260

Molecular drift of p-type dopants in doped organic semiconductors driven by an external electric field and studied by spectroscopic IR-microscopy — •Sebastian Beck^{1,2}, Vipilan Sivanesan^{1,2}, Lars Müller^{2,3}, Seon-Young Rhim^{1,2}, Jakob Bernhardt^{1,2}, and Annemarie Pucci^{1,2} — ^{1}Universität Heidelberg, Kirchhoff-Institut für Physik — ^{2}InnovationLab GmbH, Heidelberg — ^{3}TU Braunschweig, Institut für Hochfrequenztechnik

A homogeneous dopant distribution is known to be important for efficient charge transfer (CT) in doped organic semiconductors as well as the functionality of organic electronic devices. Therefore, a lot of effort is made to control the molecular composition in devices throughout the deposition process. However, during device operation an unintentional movement of charged molecules such as dopants through the layers can occur and can reduce or even destroy device performance. To further improve the understanding of these effects the implementation of new analytical methods is advised. In this study, the motion of the p-type dopant Mo(tfdCO2Me)3 in highly regioregular P3HT induced by an external electric field was studied with spectroscopic IR-microscopy. The molecular drift was identified by measuring laterally resolved IR spectra of doped layers between two electrodes before and after applying a dc field of about 2 V/micron. An analysis of the changes of the vibrational modes of the dopant molecule as well as the spectral features of the charged P3HT chains enabled an estimate of the mobility of the dopant molecules. Our results are in agreement with electrical measurements and clarify underlying processes of device fatigue.

CPP 9.11 Mon 18:00 ZEU 260

Drift of Dopants in Organic Semiconductors — •Lars Mueller[1,2,3], Seon-Young Rhim[1,3], Vipilan Sivanesan[1,3], Dongxiang Wang[1], Sebastian Beck[1,3], Annemarie Pucci[1,3], Wolfgang Kowalsky[1,2,3], and Robert Lovrincic[1,2] — [1]InnovationLab, Heidelberg, Germany — [2]Institute for High-Frequency Technology, TU Braunschweig, Germany — [3]Kirchhoff Institute for Physics, Heidelberg University, Germany

Electrical doping of organic semiconductors is widely applied to fabricate high performance organic electronic devices. The usually unwanted but still prevalent effect of dopant mobility in organic semiconductors is known for various dopant molecules in terms of diffusion towards a stable equilibrium. A mostly neglected effect is the influence of operating conditions that can cause a drift of dopants additionally to the known diffusion. We study this drift behavior and compare different dopant-host combinations, starting from Poly(3-hexylthiophen-2,5-diyl) (P3HT) doped with 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ) to larger dopant molecules and different host materials. We find a dynamic drift-process that can be utilized to deliberately create highly doped and almost undoped regions within one thin film, resulting in a spatially altered conductivity. To demonstrate the applicability, we show first data of a proof-of-principle memory device that is based on a spatially controlled dopant distribution.

CPP 10: Bioinspired Functional Materials II

Time: Monday 15:00–18:15 Location: ZEU 114

CPP 10.1 Mon 15:00 ZEU 114

Extreme refractive index wing scale beads cause the bright colors of pierid butterflies — •Bodo Wilts[1], Bas Wijnen[2], Ullrich Steiner[1], and Doekele Stavenga[2] — [1]Adolphe Merkle Institute, University of Fribourg, Switzerland — [2]University of Groningen, Groningen, the Netherlands

Butterflies feature strong, vivid colours due to photonic structures on their surface. Butterflies of the family Pieridae are brightly colored, ranging from white to red, caused by various pterin pigments concentrated in scattering spheroidal beads in the wing scales. Given the sparsity of the beads in the wing scales, the high brightness suggests a scattering strength of the beads that significantly surpasses that of typical cuticular chitin beads with the aereal density found in the wing scales. To elucidate this apparent contradiction, we have analyzed the optical signature of the pierids* highly saturated pigmentary colors by using Jamin-Lebedeff interference microscopy combined with Kramers-Kronig theory and light scattering modeling. We show that extreme pterin pigment concentrations cause a very high refractive index of the beads with values above 2 across the visible wavelength range, thus creating one of the most highly light scattering media thus far discovered in the animal kingdom.

CPP 10.2 Mon 15:15 ZEU 114

Actuated Self-(Un)rolling Silk Microstructures: Rings, Tubules, and Hhelical Tubules — •Chunhong Ye[1,2], Svetoslav V Nikolov[3], Ren Geryak[2], Rossella Calabrese[4], Alexander Alexeev[3], David L Kaplan[4], and Vladimir V Tsukruk[2] — [1]Institute of Physical Chemistry and Polymer Physics, Leibniz Institute of Polymer Research, Dresden, 01169 Germany — [2]School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332 USA — [3]Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332 USA — [4]Department of Biomedical Engineering, Tufts University, 4, Colby street, Medford, MA 02155 USA

We demonstrated facile, reversible, fast self-rolling biopolymer microconstructs using sandwiched active-passive, silk-on-silk morphology. We experimentally showed and theoretically confirmed that the shape of individual sheets effectively controls biaxial stresses within these sheets which can self-roll themselves into distinct 3D structures including microscopic rings, tubules, and helical tubules. This is a unique example of tailoring self-rolled 3D geometries though shape design without changing the inner morphology of active bimorph nanomaterials. Furthermore, the self-rolling direction, percentage shape, and diameter of the silk microtubes can be readily controlled over the geometry of the 2D microsheets, such as lateral dimension, thickness and aspect ratio. The microstructrues indicated highly reversible rolling/unrolling by alternating the external pHs, attributed to the significant swelling/deswelling of silk active layer at different pHs.

CPP 10.3 Mon 15:30 ZEU 114

Shear-induced transformation of polymer-rich lamellar phases to micron sized vesicles investigated by small-angle scattering — •Sören Grosskopf[1], Miriam Siebenbürger[2], Oliver Wrede[1], Yvonne Hertle[1], and Thomas Hellweg[1] — [1]Bielefeld University — [2]Helmholtz-Zentrum Berlin

The influence of adding an amphiphilic triblock copolymer to a cationic microemulsion results on the one hand in an increasing viscosity and on the other hand in complexer phase behavior with an enhanced lamellar phase. This is a common feature of amphiphilic block copolymers related to the *efficiency boosting effect.* The aim of this work was to fabricate multi-lamellar-vesicles (MLV) out of a triblockcopolymer-rich lamellar phase applying stress and their identifaction via small angle scattering. The system consists beside the the polymer of a polar and apolar component and an cationic co-surfactant. Such large vesicles are of potential interest for the usage as drug delivery systems. Different *rheo*-small-angle scattering techniques were used to investigate structures while applying shear stress: With neutrons the change in the bilayer spacing can be investigated. For the research of larger structures depolarized rheo-small-angle light scattering (*rheo*-SALS) was used. The *rheo*-SALS experiments shows an inverse dependency of the applied shear-rate on the size of the MLVs. Beside the small-angle scattering experiments different microscopy techniques (polarized light, difference interference contrast microscopy) was used to obtain real space pictures of the resulting particles.

CPP 10.4 Mon 15:45 ZEU 114

Carbon-Nanotube Membranes from Self-Assembly in Lipid Bilayers — •Martin Vögele, Jürgen Köfinger, and Gerhard Hummer — Max-Planck-Institut für Biophysik, Frankfurt am Main

Carbon nanotube (CNT) pores in lipid membranes are a promising candidate for applications as molecular filters and in drug delivery. The similarity of such pores to cylindrical membrane proteins raises the question whether they can self-assemble to a thin membrane with a high density of pores in a manner similar to protein 2D crystallization. We apply fully atomistic and large-scale coarse-grained molecular dynamics simulations to explore the hypothetical formation of such a material and to guide future experiments.

We find that indeed carbon nanotubes self-assemble to large clusters in lipid membranes. As the up-right carbon nanotubes induce very strong annular lipid shells around themselves, those clusters include trapped lipids between the CNTs. This trapped state is advantageous as it softens boundaries between otherwise incompatible local crystalization nuclei.

Our simulations suggest that the lipid composition is less important for the experimental procedure to produce such membranes but it will need a very subtle fine-tuning of the CNT properties. If this can be mastered, there is a broad field of applications, e.g. in desalination or dialysis, with many possibilities to tune the desired properties of the material.

CPP 10.5 Mon 16:00 ZEU 114

The impact of surface curvature on growing tissues — •Sebastian Ehrig[1], Alan West[1], Cecile M. Bidan[2], Karen Lam[1], Philip Kollmannsberger[3], Pavel Tomancak[4], Peter

Fratzl[1], and John W.C. Dunlop[1] — [1]MPIKG, Potsdam, Germany — [2]CNRS, Université Grenoble Alpes, France — [3]University of Würzburg, Germany — [4]MPICBG, Dresden, Germany

Biological tissues continuously undergo shape changes that effect the development and regeneration of tissues and organs. These changes are regulated by cells confined within a complex environment of mechanical and biochemical constraints. Cells not only respond to the geometry of their local environment but also modify it, through the production of extracellular matrix. How these cells are able to form complex tissue structures over large distances, however, is still elusive. Motivated by the observation that tissues grown on substrates of controlled curvature in-vitro are strongly influenced by the local curvature, we have performed tissue culture experiments on surfaces of constant mean curvature and are able to show that the mean curvature has a strong impact on the rate of tissue growth and on the organization of the cellular structures. We can show that on long time scales the tissue surface behaves like a viscous fluid with an equilibrium shape governed by the Laplace-Young-law. Cells on these surfaces display liquid-crystal like behaviour leading to remarkably symmetric stress patterns that closely resemble geodesics. The emergence of such patterns is a result of the intrinsic surface curvature and can partly be explained by minimizing the free energy of the cells director-field.

CPP 10.6 Mon 16:15 ZEU 114

Colloid Clusters in Confinement: Observation, Modelling and Simulation — •Junwei Wang[1,2], Michael Engel[2], and Nicolas Vogel[1] — [1]Institute of Particle Technology, Friedrich Alexander Universität, Erlangen, Germany — [2]Institute of Multiscale Simulation, Friedrich Alexander Universität, Erlangen, Germany

Natural materials evolve to maximize performance from a limited choice of simple building blocks. Structural coloration is one example where nature utilizes ordered nanostructures to create vivid color. Colloidal particles are ideal building blocks to mimic this design principle, as their sizes match with wavelength of visible light. Colloids assemble upon increase of volume fraction into crystals, driven by entropy. Recent studies show that for colloids in spherical confinement, entropy favors icosahedral symmetry. Here we experimentally realize and geometrically model highly ordered icosahedral colloid assemblies. We discuss and compare stabilization mechanisms. Our study demonstrates the ability to create sophisticated colloid assemblies via confinement, which may find use as templates, photonic materials, and building blocks for hierarchical assembly.

15 min break

CPP 10.7 Mon 16:45 ZEU 114

Nonclassical Crystallization in vivo et in vitro: origin and mimesis of a fundamental and nanoscale process-structure-property relationship of biominerals — •Stephan E. Wolf — Friedrich-Alexander-University Erlangen-Nürnberg, Erlangen, Germany; Juniorprofessor for Biomimetic Materials and Processes

Hidden within their structural wealth, a distinct nanogranular fine structure is shared by nearly all biominerals. This structural dichotomy of universality vs. diversity roots in a common nanoparticle-mediated growth, i.e. nonclassical crystallization, which underlies the formation of these nanogranular biominerals. This reveals a fundamental process-structure-property relationship of biominerals since the nanoscale organic-inorganic composite design affects multiple properties of the bioceramic. The mimesis of such a nanogranular material can be readily accomplished by exploitation of an in vitro mineralization route which involves accretion of amorphous colloids and their subsequent solid-amorphous to solid-crystalline phase transformation. This model system allows an unpreceded view on the mineral phase transformation and allows further the mimesis of crystal lattice tilting and twisting as observed in biogenic minerals. We discuss the origin of this peculiar crystallographic feature and demonstrate that crystal lattice bending represents a powerful, yet unexploited means to design and dynamically control anisotropic properties of a crystalline material. Revelation of the underlying mechanisms may pave the way to new classes of gradient materials and provide a new view on crystallographic design of solid state materials.

CPP 10.8 Mon 17:00 ZEU 114

Gyroid Optical Metamaterials: Termination-Induced Anisotropy — •Matthias Saba[1], James A. Dolan[2,4], Raphael Dehmel[2], Angela Demetriadou[1], Ilja Gunkel[5], Yibei Gu[3], Ulrich Wiesner[3], Timothy D. Wilkinson[4], Ullrich Steiner[5], Jeremy J. Baumberg[2], Bodo D. Wilts[5], and Ortwin Hess[1] — [1]Department of Physics, Imperial College, Prince Consort Road, London SW7 2BB, UK — [2]Department of Physics, University of Cambridge, J.J. Thomson Avenue, Cambridge CB3 0HE, UK — [3]Department of Materials Science and Engineering, Cornell University, 214 Bard Hall, Ithace, NY 14853-1501, USA — [4]Department of Engineering, University of Cambridge, J.J. Thomson Avenue, Cambridge CB3 0HE, UK — [5]Adolphe Merkle Institute, Ch. des Verdiers 4, 1700 Fribourg, Switzerland

Inspired by gyroid photonic crystals that are found in the wing-scales of several butterfly species, metallic gyroids fabricated via self-assembly constitute the first example of a truly three dimensional optical metamaterial. Gyroid metamaterials (GMMs) are known for their unique optical properties, such as linear and circular dichroism.

We here demonstrate experimentally and theoretically that (a) short range order GMMs essentially behave similar to isotropic nanoporous gold and can effectively be modeled by a Bruggeman approach, and that (b) the strong linear dichroism observed for long range order GMMs stems from a distinct plasmonic response at the GMM surface that breaks the cubic symmetry of the gyroid and is extremely sensitive to the specific surface termination.

CPP 10.9 Mon 17:15 ZEU 114

Immobilization Strategies for Photoactive Metal-Complexes on Carbon Nanomembranes — Maria Küllmer[1], Patrick Endres[2], Christof Neumann[1], •Andreas Winter[1], Andreas Winter[2], Benjamin Dietzek[1,3], Ulrich Schubert[2,4], and Andrey Turchanin[1,4] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena — [2]Institute of Organic Chemistry, Friedrich Schiller University Jena, 07743 Jena — [3]Leibniz Institute of Photonic Technology, 07745 Jena — [4]Jena Center for Soft Matter, Friedrich Schiller University Jena, 07743 Jena

The investigation of artificial molecular photo catalysts plays an important role in the development of novel energy sources. In this respect, the incorporation of photoactive compounds into nanomembranes is a promising approach for such applications in the field of light harvesting and electron transfer. Ruthenium-complexes are well-known photo-sensitizers and photocatalysts, which facilitate the utilization of light energy by electron transfer to/from the actual catalyst. The preparation of photoactive nanomembranes requires selective immobilization of these species on the nanomembrane surface. Here we present various immobilization strategies of ruthenium-II-photosensitizers on 1 nm thick carbon nanomembranes (CNMs). We use thiol-ene click reactions and amide-bond formation via active esters to couple the complexes to the CNM. Alternatively the metal-capturing unit was formed intrinsically by the crosslinked self-assembled monolayer units. The functionalized CNMs have been characterized by means of X-ray photoelectron spectroscopy as well as atomic force and optical microscopy.

CPP 10.10 Mon 17:30 ZEU 114

Bio-inspired photonic structures as blueprints for compact polarization converters — •Xia Wu[1], Fernando Luis Rodríguez Gallegos[2], Marie-Christin Angermann[3], Bertram Schwind[1], Helge-Otto Fabritius[4], Georg von Freymann[3], and Jens Förstner[2] — [1]Department of Chemistry, University of Paderborn, Warburger Straße 100, D-33098, Paderborn, Germany — [2]Theoretical Electrical Engineering, University of Paderborn, Warburger Straße 100, 33098 Paderborn, Germany — [3]Physics Department, University of Kaiserslautern, Erwin-Schroedinger-Strasse, 67663 Kaiserslautern, Germany — [4]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Polarization conversion is often needed in many optical applications. In nature, many species of insects have evolved photonic structures can convert the polarization state of light upon reflection[1,2]. We reveal a new type of biological polarization converter found in the scales of weevil Entimus imperialis. We show that the D-structures in (and only in) the green domains of scales (i.e. {001} lattice plane parallel to scale surface) can act as a linear polarization converter. Furthermore we show that the D-structures in green domains preserve the handedness of the incident circularly polarized light upon reflection. Inspired by this finding, we synthesized woodpile structures by direct laser writing. We show that the well-known woodpile structure has very similar polarization conversion effect like that of D-structure. References: [1] K. Zhang et al., RSC Adv. (2014) 4, 51865-51871 [2] P. Vukusic et al., Nature (2000) 404, 457

CPP 10.11 Mon 17:45 ZEU 114

Soft and Tough as well: Morphology and Functional Structure of Spider Silk — A. Markus Anton and •Friedrich Kremer — Institute of Experimental Physics I, University of Leipzig, Germany

Spider dragline silk exhibits remarkable characteristics, such as exceptional biocompatibility or high tensile strength combined with great elasticity. Its mechanical properties are based on a refined architecture on the molecular scale: Proteins with highly repetitive core motifs aggregate into nanometer-sized crystals, rich on alanine in β-sheet secondary structure, surrounded by an amorphous glycine-rich matrix. During spinning the amorphous parts are elongated, which orients both substructures and gives rise to an inherent non-equilibrium state. Thus, external stress is directly transferred to the nanocrystals, while the tendency to contract is counterbalanced by surrounding fiber structure, as demonstrated by FTIR experiments in combination with uniaxial stress [1] or hydrostatic pressure [2].

Until recently it was not possible to artificially recreate this exceptional architecture [3]. We show that wet spinning and post-treatment of a novel biomimetic protein results in fibers with a similar nanostructure and comparable toughness as the natural template [4].

[1] P. Papadopoulos et al., *Eur. Phys. J. E* **24** (2007) 193–199; [2] A. M. Anton et al., *Macromolecules* **46** (2013) 4919–4923; [3] A. Heidebrecht et al., *Adv. Mater.* **27** (2015) 2189–2194; [4] A. M. Anton et al., *Manuscript in preparation*

CPP 10.12 Mon 18:00 ZEU 114

Hyperbolic surface decorations and novel materials — •Myfanwy Evans — Mathematics Institute, TU Berlin, Berlin, Germany

Hyperbolic surfaces form the basis of a wide array of biological structure. This talk explores the mathematical construction of secondary structures, or symmetric decorations, on these surfaces as a way to construct complex entangled materials with novel physical behaviour.

CPP 11: Modelling and Simulation of Soft Matter

Time: Monday 15:00–18:15 Location: ZEU 255

CPP 11.1 Mon 15:00 ZEU 255

Scalable and fast concurrent multiscale molecular simulation with predictive parallelization schemes — •Horacio Vargas Guzman[1], Christoph Junghans[2], Kurt Kremer[1], and Torsten Stuehn[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Computer, Computational, and Statistical Sciences Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Concurrent multiscale simulation enables the study of molecular systems with different resolutions in specific subdomains of a simulation box. Modeling soft-matter and biological systems in the context of multiscale simulations are challenging research avenues which drive the permanent development of new simulation methods and algorithms. In computational terms, those methods require parallelization schemes that make productive use of computational resources for each simulation and from its genesis. Here, we introduce the dual resolution domain decomposition algorithm that is a combination of a resolution sensitive spatial domain decomposition with an initial sliding subdomain-walls procedure. The algorithm modeling is presented for dual resolution systems in terms of scaling properties as a function of the size of the low-resolution region and the high to low resolutions ratio. The algorithm competences are validated within adaptive resolution simulations, by comparing its scalability and speedup to a spatial domain decomposition. Two representative adaptive resolution simulations have been employed in this work, namely, a biomolecule solvated in water and water in an ideal gas reservoir.

CPP 11.2 Mon 15:15 ZEU 255

Controlling the Distance of Core-Shell Nanostructures via Star Polymers — •Qiyun Tang[1], Christian Rossner[2], Marcus Müller[1], Philipp Vana[2], and Otto Glatter[3] — [1]Institute für Theoretische Physik, Georg-August-Universität, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Institute für Physikalische Chemie, Georg-August-Universität, Tammannstrasse 6, D-37077 Göttingen, Germany — [3]Institute für Anorganische Chemie, Technische Universität Graz, Stremayrgasse 9/V, A-8010 Graz, Austria

Recent experiments have demonstrated that the star polymers can be used to precisely control the distance of core-shell nanostructures, which are formed by a single, large and multiple, small gold nanoparticles. Here we use a Monte Carlo simulation based on a coarse-grained bead-spring model to systematically study the distance scaling behaviour of this core-shell nanostructure. Our results show that these distances are mainly controlled by the position of free arm ends of star polymers, and the simulation results are in good agreement with the small-angle X-ray scattering (SAXS) results of core-shell nanostructures dispersed in solution. Interestingly, we found that the scaling of core shell distances for 2-arm, 3-arm, and 6-arm star polymers approaches one master curve as a function of the arm length of star polymers. We also found that increasing the arm number of star polymers could increase the density of free arm end groups, and therefore grab more small gold nanoparticles. Our results show the feasibility to precisely control the core-shell structures at the nanoscale.

CPP 11.3 Mon 15:30 ZEU 255

Formation of multicore structures in single dendritic-linear copolymers — •Martin Wengenmayr[1,2], Ron Dockhorn[1,2], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Germany — [2]Technische Universität Dresden, Germany

Dendritic polymers gain attention for promising applications in drug delivery purposes or as catalysts. Usually the dendritic part will be rather hydrophobic and has the tendency to collapse in aqueous environment. Hydrophilic chains attached to the terminal groups form a corona being reminiscent to a polymer micelle. We investigate the conformational and thermodynamic properties of these molecules by analytical models and computer simulations. A mean-field model applying the Daoud-Cotton approach and a surface tension argument is presented and suggests the splitting of the unimolecular single-core structure into a multicore structure with increasing dendrimers generation and decreasing solvent selectivity. Monte Carlo simulations utilizing the bond fluctuation model with explicit solvent are performed which show the formation of multicore structures for trifunctional codendrimers. These findings are aimed to understand the physics of spontaneous self-assembly of co-dendrimers in various well-defined macro-conformations under change of environmental conditions.

CPP 11.4 Mon 15:45 ZEU 255

Controlled Fabrication of Nanoparticles through Rapid Solvent Exchange — •Tatiana Morozova and Arash Nikoubashman — JGU, Mainz, Germany

Polymeric nanoparticles are widely sought after for scientific and technological applications, but large-scale fabrication techniques are still at an early development stage. Recently, a new technology to form monodisperse polymer nanoparticles through rapid micromixing of polymers in solution (tetrahydrofuran, THF) with a nonsolvent (water) was developed. The general applicability of this technique for the large scale fabrication of monophasic and biphasic Janus nanoparticles has been demonstrated recently [1,2], but the underlying self-assembly mechanisms are still largely unknown. To elucidate this behavior, we performed united atom molecular dynamic (MD) simulations of a single polystyrene (PS) chain in THF-water mixtures with variable mixing ratios. Depending on the mole fraction of water, the mixture is either a good or a bad solvent for PS and the polymer coil collapses into a globule. We developed appropriated force fields for these complex systems and analyzed systematically the polymer radius of gyration depending on solvent quality. These detailed simulations will allow us to develop a physically informed coarse grained model, which can be used to perform simulations with multiple chains.

[1] A. Nikoubashman, V.E. Lee, C. Sosa, R.K. Prud'homme, R.D. Priestley and A.Z. Panagiotopoulos, ACS Nano 10, 1425 (2016)

[2] C. Sosa, R. Liu, C. Tang, F. Qu, S. Niu, M.Z. Bazant, R.K. Prud'homme, R.D. Priestley, Macromolecules 49, 3580 (2016)

CPP 11.5 Mon 16:00 ZEU 255

Polymer bottlebrushes in solution: A combined theory and simulation study — Jaroslaw Paturej, •Torsten Kreer, and

Jens-Uwe Sommer — Leibniz-Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden

We present a theoretical model for polymer bottlebrushes in solutions, where the branched chain is considered as a sequence of cylindrical blobs. Our approach delivers a consistent description of backbone and side-chain scaling under variation of concentration, providing power-laws in different concentration regimes. Upon increasing concentration, we envision a hierarchical screening: First, there is screening by the cylindrical blobs of different chains. Further increase of the concentration leads to screening inside the overlapping cylinders and, finally, amongst the side chains of different brushes. Our analytical predictions are tested via molecular dynamics simulations, which reveal very good agreement with the theory.

CPP 11.6 Mon 16:15 ZEU 255

Depleted depletion drives polymer swelling in poor solvent mixtures — •Debashish Mukherji[1], Carlos Marques[2], Torsten Stuehn[1], and Kurt Kremer[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Institut Charles Sadron, CNRS, Strasbourg, France

Macromolecular solubility in solvent mixtures often strike as paradoxical phenomena [1]. In a system where all particle interactions are repulsive, chains can nevertheless collapse, due to increased repulsive monomer-solvent interactions that lead to an effective attraction between monomer units also known as depletion induced attraction. While it is well understood why a polymer can collapse in a purely repulsive solvent, polymer swelling at intermediate mixing ratios of two repulsive solvents still lacks a microscopic explanation. Here, for binary solvent mixtures, we combine computer simulations and theoretical arguments to unveil the microscopic, generic origin of this collapse-swelling-collapse scenario. We show that this phenomenon naturally emerges at constant pressure in mixtures of purely repulsive components when a delicate balance of the entropically driven depletion interactions is achieved [2]. [1] D. Mukherji, C. M. Marques, and K. Kremer, Nature Communications 5, 4882 (2014). [2] D. Mukherji, C. M. Marques, T. Stuehn, and K. Kremer, arXiv:1609.09839 (2016).

15 min break

CPP 11.7 Mon 16:45 ZEU 255

The stretching behaviour of a single tethered polymer in pressure-driven flow — •Kai Szuttor[1], Tamal Roy[2], Steffen Hardt[2], Christian Holm[1], and Jens Smiatek[1] — [1]Institute for Computational Physics, Stuttgart, Germany — [2]Centre of Smart Interfaces, Darmstadt, Germany

We incorporate mesoscopic molecular dynamics (MD) simulations to investigate the stretching behaviour of a tethered polymer in a confined geometry. In particular we are interested in the connection between fluid flow characteristics and the force on the polymer chain. In addition, the comparison to analytical predictions show that hydrodynamic interactions (HIs) are crucial for the observed stretching behaviour. However, the comparison also shows that the general scaling behaviour for the stretching is not strongly influenced by HIs. Simulation results agree with recent experimental results for λ-DNA stretching in micro scale channels.

CPP 11.8 Mon 17:00 ZEU 255

Dynamics of polymer chains in active fluids — •Jaeoh Shin and Vasily Zaburdaev — Max Planck Institutes für Physik komplexer Systeme, Dresden, Germany

While the dynamics of polymer chains in viscous fluids are well understood, the dynamics in active fluids, which are common in living systems, can be very different. Here we study the dynamics of polymer chains in fluids that contain active Brownian particles (ABPs) in 2D by using Brownian dynamics simulations. The ABPs can be trapped in concave regions of the polymer contour and thus can strongly affect the propulsion of the polymer. The polymer center of mass shows super-diffusive motion at short times and above the capturing time of the ABPs, it goes to normal diffusion with the diffusivity much larger than in the case of a passive viscous medium. Interestingly, the long time diffusivity shows a non-monotonous behavior as functions of both the chain length n and the bending stiffness κ. We analyze the chain conformation by looking at its Fourier modes and find that at the optimal length/ stiffness, the chain has preferentially bent conformations. Finally, we consider the barrier crossing of polymer chains in a double-well potential. The crossing times show a non-monotonous behavior as a function of n and κ due to the non-monotonous diffusivity. These findings can be instrumental for efficient sorting of polymer chains by their length and elastic properties.

CPP 11.9 Mon 17:15 ZEU 255

An improved dissipative coupling scheme for a system of Molecular Dynamics particles interacting with a Lattice Boltzmann fluid — •Nikita Tretyakov[1] and Burkhard Duenweg[1,2,3] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Institute for Solid State Physics, Technical University of Darmstadt, Germany — [3]Department of Chemical Engineering, Monash University, Australia

We consider the dissipative coupling between a stochastic Lattice Boltzmann (LB) fluid and a particle-based Molecular Dynamics (MD) system, as it was first introduced by Ahlrichs and Duenweg (J. Chem. Phys. 111 (1999) 8225). The fluid velocity at the position of a particle is determined by interpolation, such that a Stokes friction force gives rise to an exchange of momentum between the particle and the surrounding fluid nodes. For efficiency reasons, the LB time step is chosen as a multiple of the MD time step, such that the MD system is updated more frequently than the LB fluid. In this situation, there are different ways to implement the coupling: Either the fluid velocity at the surrounding nodes is only updated every LB time step, or it is updated every MD step. It is demonstrated that the latter choice, which enforces momentum conservation on a significantly shorter time scale, is clearly superior in terms of stability and accuracy, and nevertheless only marginally slower in terms of execution speed. The second variant is therefore the recommended implementation.

CPP 11.10 Mon 17:30 ZEU 255

Modeling Structure Formation of Twin Polymerization via a reactive Bond Fluctuation Model — •Janett Prehl and Constantin Huster — Technische Universität Chemnitz, Chemnnitz, Deutschland

Utilizing twin polymerization the formation of nanostructured organic-inorganic hybrid materials is possible in only one single reaction process. These hybrid materials consist of an interweaved organic polymer with an inorganic network. Both materials exhibit nanoporous structures at 0.5-3nm, which is a desirable property for i.e. gas storage- or fuel cell media.

Although a huge class of twin monomers triggering twin polymerization are identified and first quantum chemical calculations are performed, the structure formation process leading to the nanoporous materials as well as influence factors defining the porosity are still not known in detail. However, this knowledge would help to design customized materials for future applications.

To gain insights into the structure formation process and the resulting morphology we develop a Monte-Carlo-based reactive bond fluctuation model for twin polymerization. After introducing our model and explaining the obtained results we will also compare them with experimental data.

CPP 11.11 Mon 17:45 ZEU 255

The Wang-Landau Reaction Ensemble Method: Simulation of Weak Polyelectrolytes and General Acid-Base Reactions — •Jonas Landsgesell — ICP Uni Stuttgart, Stuttgart, Deutschland

We present a novel method for the study of weak polyelectrolytes and general acid-base reactions in molecular dynamics and Monte Carlo simulations. The approach combines the advantages of the reaction ensemble and the Wang-Landau sampling method. Deprotonation and protonation reactions are simulated explicitly with the help of the reaction ensemble method while the accurate sampling of the corresponding phase space is achieved by the Wang-Landau approach. The combination of both techniques provides a sufficient statistical accuracy such that meaningful estimates for the density of states and the partition sum can be obtained. With regard to these estimates, several thermodynamic observables like the heat capacity or reaction free energies can be calculated. We demonstrate that the computation times for the calculation of titration curves with a high statistical accuracy can be significantly decreased when compared to the original reaction ensemble method. The applicability of our approach is validated by the study of weak polyelectrolytes and their thermodynamic properties.

CPP 11.12 Mon 18:00 ZEU 255

Studying multicomponent polymer solutions with a particle-based model linked to simple density functional theory — •Jianguo Zhang, Debashish Mukherji, Kurt Kremer, and

Kostas Daoulas — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Multicomponent polymer solutions are fascinating systems for polymer physics, due to complex structural, thermodynamic, and rheological properties. Molecular-level mechanisms controlling these properties are only partially understood, which complicates technological applications, e.g. coating processes. This knowledge gap motivates our study, where we investigate ternary (polymer, solvent, cosolvent) mixtures using a mesoscopic particle-based model. Polymers and (co)solvent molecules are described [1] as worm-like chains and single beads, respectively. Non-bonded interactions are introduced through a polynomial functional, which is third order in local component densities. Analytical mean-field results for equations-of-state and compressibility facilitate the parameterization of the model. The functional-based definition serves as a framework for Monte Carlo simulations using a simple particle-to-mesh scheme. Different scenarios for polymer solubility in solvent and cosolvent are considered. In the dilute regime, the model reproduces co-non-solvency behavior observed previously with a generic microscopic model [2]. Conformational and structural properties at different concentrations are studied, modeling polymer films exposed to solvent-cosolvent vapor at different partial pressures. [1] Zhang et al, EPJ SP 2016. [2] Mukherji et al, Nat Commun 2014.

CPP 12: Focus: Soft Particles in Flows II (joint focus session CPP/DY)

Organized by S. Gekle, G. Gompper, C. Wagner

Time: Monday 15:00–18:00 Location: ZEU 160

Invited Talk CPP 12.1 Mon 15:00 ZEU 160

Particle alignment in microchannels and microjets — •Stephan Foerster[1], Mathias Schlenk[1], Susanne Seibt[1], Martin Trebbin[3], Josef Breu[1], and Stephan Roth[2] — [1]University of Bayreuth, Bayreuth, Germany — [2]DESY, Hamburg, Germany — [3]University of Hamburg, Hamburg, Germany

The flow orientation of particles in microflows is of high relevance in many areas ranging from synthetic fiber production to streams of cells and proteins in blood capillaries. With current advances in device miniaturization in microfluidics, X-ray optics and high-resolution optical microscopy, it has become possible to study the flow orientation of anisometric colloids in-situ with unprecedented precision.

We investigated the flow orientation of Au-nanorods, wormlike polymer micelles and hectorite nanosheets in curved and tapered microchannels. We sursprisingly find that all anisometric particles align perpendicular to the flow orientation in the widening section of tapered microchannels. This is caused by strong extensional forces that reorient the particles. This phenomenon is even observed during the formation of microdroplets from microjets, resulting in biaxial orientations of particles in the free droplets. These findings have important consequences for the production of high performance fibers and the agglomeration of particles in blood capillary stenoses.

CPP 12.2 Mon 15:30 ZEU 160

Intricate dynamics and morphology of red blood cells under physiological flow conditions — Johannes Mauer[1], Luca Lanotte[2], Simon Mendez[3], Viviana Claveria[2], Franck Nicoud[3], Manouk Abkarian[2], Gerhard Gompper[1], and •Dmitry A. Fedosov[1] — [1]Institute of Complex Systems, Forschungszentrum Juelich, 52425 Juelich, Germany — [2]Centre de Biochimie Structurale, CNRS UMR 5048, University of Montpellier, 34090 Montpellier, France — [3]Institut Montpellierain Alexander Grothendieck, UMR5149, University of Montpellier, 34095 Montpellier, France

Red blood cells (RBCs) constitute the major cellular part of blood. They have a biconcave shape with a membrane consisting of a lipid bilayer with an attached cytoskeleton formed by a network of the spectrin proteins. The RBC membrane encloses a viscous cytosol (hemoglobin solution), so that RBCs possess no bulk cytoskeleton and organelles. Despite this simple structure, RBCs exhibit fascinating behavior in flow showing complex deformation and dynamics. Current simplified understanding of RBC behavior in shear flow is that they tumble or roll at low shear rates and tank-tread at high shear rates. This view has been mainly formed by a number of experiments performed on RBCs dispersed in a viscous solution, which is several times more viscous than blood plasma. However, under physiological conditions with increasing shear rates, RBCs successively tumble, roll, deform into rolling stomatocytes, and finally adopt highly-deformed poly-lobed shapes. This behavior is governed by RBC elastic and viscous properties and it is important to consider it under relevant physiological conditions.

CPP 12.3 Mon 15:45 ZEU 160

Red blood cells in high shear and strain rates: how numerical simulation can contribute — •Simon Mendez, Etienne Gibaud, and Franck Nicoud — IMAG, UMR CNRS 5149, University of Montpellier. 34095 Montpellier. France

Red blood cells (RBCs) constitute 99 percent of the formed elements present in blood. The dynamics of RBCs controls the complexity and the behavior of blood itself, as red blood cells constitute approximately 40 percent of the whole blood volume. The individual dynamics of a RBC is still a topic of research. This is particularly the case at high shear and strain rates, for which experimental data are scarce, due to the difficulty of visualizing the RBC dynamics in high-speed flows.

Although computing the RBCs dynamics in flows with high shear/strain rates is challenging, numerical simulation does not suffer from the same limitations as in vitro experiments of high-speed flows. This talk will illustrate how computations can be used in this context to gain new insight in the dynamics of red blood cells.

Two examples will be used: the behavior of RBCs at high shear rate in a low-viscosity fluid and the dynamics of RBCs during their counting and sizing in industrial blood analyzers, where strain dominates.

CPP 12.4 Mon 16:00 ZEU 160

Structure and dynamics of colloidal short range repulsive interacting suspensions with weak attractive interactions. — Clara Weis and •Norbert Willenbacher — Karlsruhe Institute for Technology, Karlsruhe, Germany

The effect of weak attractive interactions on structure and dynamics of aqueous polymer dispersions is investigated using Multiple Particle Tracking (MPT) and classical rotational rheology. This allowed us to correlate microstructure, structural heterogeneities and local particle mobility in fluid, fluid/crystalline, glassy and gel like samples with the corresponding macroscopic flow behavior. For volume fractions $\phi <$ 0.5 good agreement between micro- and macro-viscosity was found. As weak attractive interactions were induced by adding non-adsorbing polymer, an enormous broadening of the fluid-crystalline co-existence regime was observed. MPT allowed for retrieving the phase composition, i.e. the fraction of the fluid and crystalline regions as well as the respective particle concentration, completely. In addition, the size of the crystals as well as their shear modulus could be determined. Further increasing attraction strength a gel state occurred and MPT disclosed a heterogeneous structure resembling a percolating network. At $\phi > \phi_{glass}$, the introduction of weak attractive interactions leads to a much broader fluid regime than predicted by MCT. At a given ϕ, stronger attractive interaction is required to form an attractive gel than for true hard sphere systems. MPT enables to study particle localization and structural heterogeneities on feasible, short time scales since a large number of dispersed particles are in the field of view.

CPP 12.5 Mon 16:15 ZEU 160

An iterative solution algorithm for actively and passively swimming elastic capsules — •Horst-Holger Boltz[1,2] and Jan Kierfeld[2] — [1]Institut für nichtlineare Dynamik, Fakultät Physik, Georg-August-Universität Göttingen, Göttingen, Deutschland — [2]Fakultät Physik, Technische Universität Dortmund, Dortmund, Deutschland

Soft elastic capsules which are subject a viscous fluid flow undergo shape deformation coupled to their motion. We introduce an iterative solution scheme which couples hydrodynamic boundary integral methods and elastic shape equations to find the stationary axisymmetric shape and the velocity of an elastic capsule moving in a viscous fluid at low Reynolds numbers. We use this approach to systematically study dynamical shape transitions of capsules with Hookean stretching and bending energies and spherical rest shape sedimenting under the influence of gravity or centrifugal forces [Phys. Rev. E **92**: 033003 (2015)]. Additionally, we discuss the application to actively swimming ("squirming") capsules.

15 min. break

CPP 12.6 Mon 16:45 ZEU 160

Shapes and interaction of microcapillary RBC flow — •Alexander Kihm[1], Achim Guckenberger[2], Stephan Gekle[2], and Christian Wagner[1] — [1]Saarland University, Saarbrücken, Germany — [2]Bayreuth University, Bayreuth, Germany

We try to establish the phase diagram of Red Blood Cells (RBC's) flowing through a capillary, i.e. characterize their shape and position as a function of capillary dimensions and imposed flow rate (pressure drop).

Therefore, we perform microfluidic experiments, either with a simple inverted brightfield microscope or with a recently developed 3-D confocal spinning disk technique. In most cases we find a migration of cells towards the center, but above a critical flow rate off-centered positions are observed as well. In addition, we classify the shapes of flowing cells, and as categories we distinguish between slippers, croissants and other (ambiguous) shapes. The experimental data is compared to predictions obtained from numerical simulations using a boundary-integral method.

CPP 12.7 Mon 17:00 ZEU 160

Red blood cells dynamics in biomimetic submicron splenic slits — •Annie Viallat[1], Emmanuele Helfer[1], Anne Charrier[1], Priya Gambhire[1], Scott Atwell[1], Catherine Badens[2], and Cecile Iss[1] — [1]Aix Marseille Univ, CNRS CINAM, Marseille, France — [2]Aix Marseille Univ., INSERM, GMGF, Marseille, France

In drug delivery, cancer cell dissemination and red blood cells (RBCs) splenic filtration, nanoparticles and cells have to deform and pass through the submicron and high aspect ratio gaps between the endothelial cells lining blood vessels. The dynamics of passage of particles/cells remain poorly understood because costly technologies are required to reproduce gaps of physiological dimensions in devices suitable for in-vitro optical-microscopy observations. Here, novel microfluidic PDMS devices containing high aspect ratio slits with submicron width were molded on silicon masters by using a simple, inexpensive, and highly flexible combination of standard UV lithography and anisotropic wet etching. These devices revealed novel modes of deformations of healthy and sick RBCs squeezing through slits replicating splenic slits (0.8x2x5 microns) under physiological interstitial pressures. At the slit exit the cytoskeleton of spherocytic RBCs was spectacularly detached from the lipid membrane whereas RBC shapes from healthy donors and patients with sickle cell disease exhibited peculiar tips at their front. These tips disappeared much slower in patients cells, allowing to estimate a threefold increase in RBC cytoplasmic viscosity in sickle cell disease. Measurements of both time and rate of RBC sequestration in the slits allowed quantifying the massive spherocytic RBCs trapping.

CPP 12.8 Mon 17:15 ZEU 160

Non-inertial lift and its application to label-free microfluidic cell separation and sorting — T M Geislinger[1,2], M Stamp[1], B Eggart[1], S Braunmüller[1], L Schmid[1], S Chan[2], M Koll[2], M Wahlgren[2], A Wixforth[1], and •T Franke[1,3] — [1]Experimental Physics I, University of Augsburg, 86159 Augsburg, Germany — [2]Department of Microbiology, Tumor and Cell Biology, Karolinska Institutet, Box 280, S-171 77 Stockholm, Sweden — [3]Chair of Biomedical Engineering, University of Glasgow, Oakfield Avenue, G12 8LT, Glasgow, Scotland

Reliable cell separation and sorting are important tasks in everyday's laboratory work and of increasing importance in various medical diagnoses. Widely used methods like fluorescence or magnetically activated cell sorting (FACS, MACS), however, require labelling of samples with adequate markers and/or the generation of external fields. Apart from the dimensions and the costs of such devices, any unwanted alterations of the cells by the markers potentially interfere with subsequent processes such as genetic analyses. Here, we present a simple and cheap microfluidic approach for continuous, passive and label-free cell sorting that relies on the exploitation of a hydrodynamic effect for separation: the non-inertial lift effect. The non-inertial lift effect is a repulsive cell-wall interaction of purely viscous origin that acts on non-spherical and deformable objects in laminar flow fields. Generally, the lateral drift becomes stronger for larger and more deformable objects. We examine this effect for separation of different cells including circulating tumor cells and malaria infected red blood cells.

CPP 12.9 Mon 17:30 ZEU 160

Jammed capsules as a model system for soft glassy matter — •Othmane Aouane[1], Andrea Scagliarini[1], and Jens Harting[1,2] — [1]Forschungszentrum Jülich, Helmholtz Institute Erlangen-Nürnberg, Nürnberg, Germany — [2]Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands

Soft-glassy materials describe materials exhibiting a solid-like behavior at rest and local yielding when subject to a high enough stress. While systems like foams, emulsions[1], colloidal and polymer gels have been widely studied in the last decades; still a little is known about the flow behavior of deformable microgels. We investigate numerically the rheology of microgels formed by dense suspensions of capsules under mechanical stress in an athermal system. In a first step, the packing of capsules is done by increasing the size of the scaled deformable particles until reaching the desired size meanwhile the dynamical evolution of the system follows a molecular dynamics-like approach. After the initialization stage and the formation of the microgel structure, we use the lattice Boltzmann method to resolve the fluid motion and the immersed boundary method to couple between the finite element capsules and the fluid [2]. We investigate the existence or not of local yield points by varying the concentration of capsules from 60 to 90%. The effect of elasticity and mechanical forcing are also considered in our study.

[1] Benzi, R., *et al.* Europhysics Letters, 104.4 (2013): 48006

[2] Krüger, T., *et al.* Journal of Fluid Mechanics, 751 (2014): 725-745

CPP 12.10 Mon 17:45 ZEU 160

Dynamics of microcapsules in elongational and shear flows — •Clement de Loubens[1], Kaili Xie[2], and Marc Leonetti[3] — [1]Laboratoire Rheologie et Procedes, Grenoble, France — [2]M2P2, Marseille, France — [3]IRPHE, Marseille, France

A capsule is a drop bounded by a thin solid membrane providing specific mechanical properties. The interfacial rheological properties of these soft microparticles are deduced from their dynamics of deformation in elongational and shear flows.

In elongational flow, the surface shear modulus of the membrane is measured and related to the kind of biopolymer used and to the main parameters of the process of fabrication. In the regime of large deformations, the microcapsules can present a non-linear elastic response or plastic deformations. Non-linear elastic constitutive law is deduced by comparison of the evolution of the shape of the microcapsule in the two main planes of deformation of the capsule with numerical simulations.

In shear flow, the rotation of the membrane, i.e. the tank-treading, is visualised and quantified by decorating the membrane of microcapsules with particles. The tracking of the distance between two close microparticles showed membrane contraction at the tips and stretching on the sides. This dynamics of deformation induce viscous dissipation inside the membrane. The order of magnitude of membrane viscosity is determined by comparison with numerical simulations.

We will conclude the talk by some examples of breakdown of microcapsules in elongational flow.

CPP 13: Poster: Fundamentals of Perovskite Photovoltaics (joint session CPP, DS, HL)

Time: Monday 18:30–21:00 Location: P1A

CPP 13.1 Mon 18:30 P1A

Hybrid photovoltaics based on diblock copolymer structured, mesoporous Ge thin films — •Andreas Hetzenecker[1], Nuri Hohn[1], Michael Giebel[2], Thomas F. Fässler[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]TU München, Chemie-Department, LS Anorganische Chemie mit Schwerpunkt Neue Materialien, Lichtenbergstr. 4, 85748 Garching

Hybrid photovoltaics opens new possibilities in solar cell design, combining the mechanical stability and high charge carrier mobility of semiconductors with the potentially cost-efficient, large scale production and flexibility of organic materials. The usage of poly(styrene-b-ethylene oxide) as a template and K_4Ge_9 Zintl clusters as an inorganic precursor [1] for sol-gel synthesis is a novel approach to produce mesoporous germanium structures. This method offers control over pore size and degree of porosity via the block lengths of the template and the reactant concentrations. Sponge-like germanium thin films were synthesized and characterized regarding their absorption behavior with UV/Vis spectroscopy. Structural analysis was performed via SEM and profilometry.

[1] M. M. Bentlohner et al., Angewandte Chemie International Edition, 55, 2441-2445 (2015).

CPP 13.2 Mon 18:30 P1A

Ultrafast charge and exciton dynamics in $CH_3NH_3PbI_3$ — •Kestutis Budzinauskas[1], Yajun Gao[1], Elina Patsikatheodorou[1], Tobias Schneider[2], Selina Otlhof[2], Klaus Meerholz[2], and Paul H.M van Loosdrecht[1] — [1]University of Cologne, II physics institute — [2]University of Coglogne, Institute of chemical physics

Solar cells based on organic-inorganic perovskite semiconductors show a surprisingly high conversion effciency. Despite tremendous progress in the field of perovskite based devices, the fundamental photophysics responsible for the good performance are still not well understood. In order to obtain a better insight of the charge separation and recombination dynamics in these materials we have performed ultrafast time resolved absorption experiments in the VIS/NIR spectral range on pure $MAPbI_3$ (CH_3 NH_3PbI_3) films, as well as on multilayer systems which use PEDOT:PSS and $PC_{61}BM$ as charge selective extraction layers. Our experiments allow to selectively monitor diffusion and recombination processes as well as interfacial charge transfer and the formation of interfacial charge transfer states with a sub-100 fs time resolution

CPP 13.3 Mon 18:30 P1A

Ultrafast charge and exciton dynamics in $CH_3NH_3PbI_3$ — •Kestutis Budzinauskas[1], Yajun Gao[1], Elina Patsikatheodorou[1], Tobias Schneider[2], Selina Otlhof[2], Klaus Meerholz[2], and Paul H.M. van Loosdrecht[1] — [1]University of Cologne, II physics institute — [2]University of Cologne, Institute of chemical physics

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CPP 13.4 Mon 18:30 P1A

morphology evolution of titania films during in situ spray coating for perovskite solar cells — •Bo Su[1], Herbert A. Caller-Guzman[1], Volker Körstgens[1], Yichuan Rui[2], Yuan Yao[1], Stephan V. Roth[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]College of Chemistry and Chemical Engineering, Shanghai University of Engineering Science, Shanghai 201620, P. R. China — [3]DESY, Notkestr. 85, 22607 Hamburg, Germany

We combine a sol-gel route with spray coating to obtain porous titania films. Spray coating is used as deposition method since it is allowing for scaling-up to large scale production. A block copolymer template assisted sol-gel process is used to form nanostructured titania films. The structure evolution is probed with in situ GISAXS during the spray coating process, enabling the detection of characteristic length scales during fabrication. The morphology of the sprayed films is characterized ex-situ with SEM, TEM and optical microscopy as well. In addition, the crystalline structure of the titian films is probed with XRD. The perovskite solar cells based on sprayed titania films are characterized under AM 1.5G standard condition. We extract a structure-function relationship for different spray parameters.

CPP 13.5 Mon 18:30 P1A

Influence of processing parameters on the morphology of perovskite solar cells — •Armin Schreiber, Johannes Schlipf, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Over the last decade, especially lead halide perovskites as an organic-inorganic hybrid compound received attention due to the exceptional rise in the power conversion efficiency (PCE) of research cells from 3.8 % in 2009 to more than 20 % in early 2016. The most common active layer material is methylammonium lead iodide ($MAPbI_3$). It can be fabricated using a solution conversion method consisting of firstly spin-coating lead iodide (PbI_2) and secondly immersing it in a solution of dissolved methylammonium iodide. This leads to strong preferential crystal orientations as evidenced by grazing-incidence small angle X-ray scattering (GIWAXS) measurements. The crystal orientation is tunable via temperature variation of precursors of the perovskite and the use of additives into the precursor or conversion solution [1]. We expand this study by the use of mixed solvent approaches with processing additives in order to further tune the time scales of the crystallization processes and gain more control of the film morphologies of perovskite thin films as well as improving the reproducibility and long-term stability.

[1] L. Oesinghaus et al., Adv. Mater. Interfaces 2016, 1600403

CPP 13.6 Mon 18:30 P1A

Morphology of Perovskite-Based Hybrid Solar Cells — •Kiran Mathew John, Johannes Schlipf, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Organometal halide perovskites, have been shown to be great candidates for photovoltaics, owing to the strong solar absorption and the high mobility and low recombination rates of photo-generated charge carriers in these compounds. Subsequently, solar cells made from perovskites have reached efficiencies of more than 20%, making them comparable with commercially available silicon solar cells. The performance of the perovskite cells greatly depend on their crystal morphology. We fabricate and characterise different cells by varying processing parameters including film deposition methods, annealing temperature and solvent media. By means of X-ray scattering methods, we gain insight into the inner film morphology and thus are able to correlate morphology and photovoltaic performance, with the target to get better fundamental understanding.

CPP 13.7 Mon 18:30 P1A

Polarisation resolved optical spectroscopy of single CsPbI3 nanocrystals — •Mirko Goldmann[1,2], Daniela Täuber[1,5], Juanzi Shi[1], Junsheng Chen[3], Maria E. Messing[4,5], Kaibo Zheng[3], and Ivan G. Scheblykin[1,5] — [1]Single molecule spectroscopy group, Lund University, Sweden — [2]TU Ilmenau, Germany — [3]2D spectroscopy group, Lund University, Sweden — [4]Solid State Physics, Lund University, Sweden — [5]NanoLund, Lund University, Sweden

Semiconducting metal halide nanocrystals are promising candidates for optoelectronic devices due to their high quantum yield and solution processability. Fully inorganic $CsPbI_3$ is more stable than $CH_3NH_3PbI_3$. Polarization resolved optical spectroscopy of single $CsPbI_3$ nanocrystals probes their cubic crystal structure and sperical shapes. Photoluminescence emission from freshly synthesized $CsPbI_3$ nanocrystals was found to be almost unpolarized. Several weeks old nanocrystals showed an increased appearance of polarized photoluminescence in agreement with the observation of elongated crystal shapes by TEM.

CPP 13.8 Mon 18:30 P1A

Gold cluster growth kinetics at the metal-polymer interface of water-processed hybrid solar cells studied by in-situ GISAXS sputter deposition — •Adrian Haussmann[1], Volker Körstgens[1], Franziska Löhrer[1], Martin Wörle[2], Hristo Iglev[2], Reinhard Kienberger[2], Matthias Schwartzkopf[3], Alexander Hinz[4], Oleksandr Polonskyi[4], Thomas Strunskus[4], Franz Faupel[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]TU München, Physik-Department, LS Laser- und Röntgenphysik, James-Franck-Str. 1, 85748 Garching — [3]DESY, Notkestr. 85, 22607 Hamburg — [4]CAU Kiel, Institut für Materialwissenschaft, Kaiserstr. 2, 24143 Kiel

In this work the metal-polymer interface between gold contact and active layer of water-processed hybrid solar cells is investigated. The active layer consists of an aqueous soluble polythiophene and laser-ablated titania nanoparticles. Gold sputter deposition is applied to the active layer. To obtain full information of gold cluster growth kinetics during sputter process, in-situ time resolved grazing incidence small angle X-ray scattering (GISAXS) experiments and grazing incidence wide angle X-ray scattering (GIWAXS) are carried out. Different growth regimes of gold clusters are observed from the GISAXS and GIWAXS data analysis and discussed.

CPP 13.9 Mon 18:30 P1A

Reduction of Hysteresis through PCBM in Planar Perovskite Solar Cells — •Yu Zhong[1], Carlos Andres Melo Luna[2], Richard Hildner[2], Cheng Li[1], and Sven Hüttner[1] — [1]Organic and Hybrid Electronics, Macromolecular Chemistry I, University of Bayreuth — [2]Experimental Physics IV, University of Bayreuth, Germany

Despite the development of organometal perovskite in solar cells, some problems still restrict its large-scale industrial application. Among these questions, it is urgent to address the hysteresis to realize highly efficient and reliable perovskite solar cells (PSC). The hysteresis is the discrepancy between two voltage-sweeping directions when performing a current-voltage (J-V) measurement. To suppress hysteresis, the introduction of [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) in the planar PSC has proved as an effective way. However, there is still no comprehensive understanding on it, which is the topic of this poster.

Evidences consistently show that the iodide ion migration is critical for the hysteresis behavior. Herein, we employ PL microscopy to in-situ investigate the ion migration process. By comparing the mobility of the ions in perovskite films with and without PCBM, it shows the decrease of ionic migration velocity when PCBM molecules are involved. Furthermore, temperature-dependent J-V measurements show that the activation energy of iodide ions increases in presence of PCBM molecules. Our experiment suggests that PCBM molecules passivate the iodide related defects and reduce the migration of iodide ions, thus suppressing the hysteretic behavior in PSC.

CPP 13.10 Mon 18:30 P1A

Impact of additional PbI_2 and the grain size on optical properties in hybrid lead halide perovskites — •Tobias Meier[1], Fabian Panzer[1,2,3], Tanaji Gujar[4], Mukundan Thelakkat[4], and Anna Köhler[1,2] — [1]Experimental Physics II — [2]Bayreuth Institute of Macromolecular Research (BIMF) — [3]Department of Functional Materials — [4]Applied Functional Polymers, Macromolecular Chemistry, University of Bayreuth, 95440 Bayreuth, Germany

Hybrid lead halide perovskites are a promising candidate for the absorbing layer in solar cells due to their excellent optical properties i.e. a direct band gap, a high absorption coefficient throughout the entire visible spectrum and a low exciton binding energy. It is known that the precise stoichiometry of the additives during film preparation is important for the device performance. For example a small amount of typically 10% extra PbI_2 was found to be beneficial for the performance. However, the mechanism of how incorporations of additional PbI_2 influences the optical and electronic properties and the role of grain boundaries are not completely understood yet. We therefore performed temperature dependent steady-state absorption and photoluminescence spectroscopy to investigate the impact of additional PbI_2 and the grain size on the fundamental optical properties in thin films of $CH_3NH_3PbI_3$.

CPP 13.11 Mon 18:30 P1A

Tuning the pore size of mesoporous titania films for hybrid solar cells — •Steffen Schlosser, Nuri Hohn, Lorenz Biessmann, Senlin Xia, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str 1, 85748 Garching

Hybrid solar cells combine the mechanical stability of inorganic and the versatility of organic semiconductors. Due to their potential for large-scale application, hybrid solar cells are especially interesting for low-cost industrial production. As an inorganic compound, mesoporous titania films are common for application in high-efficiency hybrid solar cells. The mesoporous character offers a high interfacial contact with the organic surfactant, usually a conjugated polymer. Challenges concerning these cells arise due to the difficulty of controlling their nanoscale structure, which affects conductivity and degree of backfilling. We focus on the tuning of the pore size of mesoporous titania nanostructures and its impact on the infiltration of the polymeric compound. Tuning of the pore sizes provides the possibility of enhancing the backfilling and thus has a positive impact on solar cell performance. In our experiments, a solution composed of an amphiphilic block copolymer and a precursor dissolved in an organic solvent is applied as a film. Immersion in an antisolvent leads to a structure formation process in the composite film, so that after calcination, a mesoporous titania film is obtained. Depending on the parameters used, the pore size can be controlled.

CPP 13.12 Mon 18:30 P1A

Scanning force microscopy on perovskites — Ilka M. Hermes[1], Victor W. Bergmann[1], Dan Li[1], Alexander Klasen[1], Simon Bretschneider[1], Markus Mezger[1,2], Rüdiger Berger[1], Wolfgang Tremel[2], and •Stefan A.L. Weber[1,2] — [1]Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [2]Johannes Gutenberg University, 55128 Mainz, Germany

In perovskite solar cells, nanoscale structures can have a huge impact on the device performance. For understanding this interplay, electrical scanning force microscopy (SFM) methods can correlate the nanoscale morphology with various surface properties: electrical conductivity (conductive SFM), surface potential in Kelvin probe force microscopy, (KPFM) or electromechanical coupling in piezoresponse force microscopy (PFM). This poster provides an overview on our activities in SFM on perovskite films and solar cells. We used KPFM to map the potential distribution on cross sections of perovskite solar cell devices in dark and under illumination, revealing distinct differences in the charging dynamics at different interfaces [1,2]. With PFM on micron-sized perovskite grains we observed a periodically alternating structure reminiscent of ferroelastic domain patterns [3]. Using a SFM under controlled humidity, the effects of reversible hydration in perovskite films on the morphology were studied [4]. Such experiments provide valuable information for the optimization of the light harvesting abilities in these materials and the fabrication processes. [1] Nat. Comm. 2014, 5. [2] ACS AM&I, 2016, 8 (30), 19402. [3] J. Phys. Chem. C (2016), 120, 5724. [4] J. Phys. Chem. C, 2016, 120 (12), 6363.

CPP 13.13 Mon 18:30 P1A

Investigating the organometal halide perovskite crystallization in mesoscopic hole-conductor-free perovskite solar cells — •Oliver Filonik[1,2], Jia Haur Lew[2], Anish Priyadarshi[2], Nripan Mathews[2], and Eva M. Herzig[1] — [1]TU München, Munich School of Engineering, Herzig Group, 85748 Garching, Germany — [2]School of Materials Science and Engineering, Nanyang Technological University, Nanyang Avenue, Singapore 639798, Singapore

Organometal halide perovskite based solar cells have emerged as the fastest-advancing photovoltaic technology to date, reaching certified solar cell efficiencies of up to 22.1%. Recently, the focus of research broadened beyond high efficiencies to key values like prolonged device lifetime and stability that are required for industrial implementation. A novel perovskite cell architecture utilizing a mesoporous scaffold with embedded perovskite addresses these challenges and is furthermore adaptable for industrial scale production. However, little is known about the perovskite crystal formation in mesoscopic scaffolds.

In this project, we fabricate a mesoscopic scaffold comprised of a mesoporous triple-layer of titania, zirconia and carbon by screenprinting and are investigating the influence of the processing additive 5-

ammonium valeric acid iodide (5-AVAI) on the perovskite solution infiltration and perovskite crystallization. Hereby, our results grant us a better understanding of the perovskite crystallization processes in a mesoscopic scaffold and are of key importance for further developments.

CPP 13.14 Mon 18:30 P1A

Fabrication and Characterization of Mesoscopic Perovskite Solar Cells — •Margret Eva Thordardottir[1,2], Oliver Filonik[1], Peter Müller-Buschbaum[2], and Eva M. Herzig[1] — [1]TU München, Munich School of Engineering, Herzig Group, 85748 Garching, Germany — [2]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Photovoltaic solar cells have been regarded as a promising energy conversion method to keep up with the worlds increasing energy consumption. Organic solar cells yield promising prospects due to their low cost fabrication, light weight and mechanical flexibility. However, the efficiency of organic solar cells are inferior to commercial silicon solar cells. Organometal halide perovskite solar cells are a product of combining the advantages of organic and inorganic systems. The steep rise of the efficiency makes them the fastest-advancing solar cell technology to date. Properties of the perovskite material like large carrier diffusion lengths, high charge-carrier mobilities and low exciton binding energy all contribute to superior performance.
In this work, we fabricated mesoscopic perovskite solar cells by using a screenprinter. We analyze processing parameters and investigate the influence on the efficiency of the solar cell. To obtain fully printed solar cells, slot die coating is compared to drop casting of the perovskite materials onto the printed layers.

CPP 13.15 Mon 18:30 P1A

Two-Photon Photoluminescence from Quantum-Dot-Like Perovskite Nanocubes — •Alexander Biewald[1,2], Veit Giegold[1,2], Richard Ciesielski[1,2], Fatma Meltem Aygüler[1,2], Nicolai Friedrich Hartmann[1,2], Pablo Docampo[3], and Achim Hartschuh[1,2] — [1]LMU Munich, Department Chemie and CeNS, 81377 Munich — [2]Nanosystems Initative Munich, 80799 Munich — [3]Newcastle University, Newcastle upon Tyne, UK

Perovskites are a promising material class for new solar cell and LED applications. Especially perovskite nanocubes, with sizes below 10 nm, are interesting because they exhibit quantum confinement which allows for tuning their optical transition energies similar to other inorganic semiconducting nanocrystals. We investigated the photoluminescence (PL) of individual $CsPbBr_3$ nanocubes deposited on glass upon pulsed two-photon excitation. Our setup combines a scanning confocal microscope and a pulse shaper in 4f geometry for amplitude and phase shaping of sub-20 fs laser pulses. We found that individual nanocubes show pronounced PL blinking, which we investigated in detail with respect to the characteristic on- and off-times. We also confirmed the non-linear intensity dependence of the PL that provides the basis for the coherent control of two-photon absorption in single nanocubes.

CPP 13.16 Mon 18:30 P1A

Investigation of planar perovskite solar cells by means of electrical impedance spectroscopy — •Markus Jakob[1], David Kiermasch[1], Mathias Fischer[1], Phillip Rieder[1], Andreas Baumann[2], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern) Bayern, 97074 Würzburg

Hybrid organic-inorganic perovskites have been recognized as a promising material for photovoltaic devices and became a hotspot in this research field over the last years. Toward the common goal of developing more efficient and stable devices better insight into the working principles is required. The interface between the crystalline perovskite and the charge selective layer has been found to be a crucial factor for the solar cell device performance. An accumulation of charged particles, either charge carriers or ions at the interface may lead to extraction barriers leading to a decrease in the overall efficiency. We investigate highly efficient solution processed perovskite solar cells in planar configuration by means of electrical impedance spectroscopy. The cells are fabricated with the well-known two step interdiffusion method using PbI_2 and CH_3NH_3I. We discuss our results for different device configurations and transport materials to identify their impact on the dielectric properties.

CPP 13.17 Mon 18:30 P1A

Transient absorption spectroscopy of hole transport materials for perovskite solar cells — Jonas Hölzer, Johannes Klein, Mirko Scholz, Thomas Lenzer, and •Kawon Oum — Universität Siegen, Physikalische Chemie, Adolf-Reichwein-Str. 2, 57076 Siegen

Perovskite-based photovoltaic devices consist of multilayer arrangements containing mesoporous TiO2, an organic-inorganic perovskite and a hole transport material (HTM) as central elements. We present a steady-state and time-resolved UV-Vis-NIR absorption study of such devices featuring different triarylamine-based HTMs, enabling us to quantify the efficiency and time scale of the hole transfer process. In addition, direct photoexcitation of the HTMs on mesoporous TiO2 and Al2O3 thin films and in different organic solvents is investigated to understand their photophysics. They exhibit photoinduced electron injection into TiO2 and form radical cation-radical anion pairs on Al2O3 by exciton-splitting. Implications of these processes for the performance of HTMs in photovoltaic devices will be discussed.

CPP 13.18 Mon 18:30 P1A

Investigation of the photophysical properties of methylammonium lead halide perovskite solar cells by electroluminescence spectroscopy — •Simon Berger[1], Philipp Rieder[1], David Kiermasch[1], Mathias Fischer[1], Kristofer Tvingstedt[1], Andreas Baumann[1,2], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research ZAE, 97074 Würzburg

Organo lead halide perovskite solar cells are in the focus of current research as one of the most promising materials in thin film photovoltaics. With many cell configurations being presented so far, we evaluated solution-processed planar as well as mesoporous perovskite solar cells in terms of their corresponding ability to emit light, using the technique of electroluminescence spectroscopy. In that manner, we probed the impact of different transport materials in regular as well as inverted layouts by evaluating the radiative efficiency of devices. Additionally, we studied the effect of incorporating bromine as well as chlorine to partly replace the iodine in the crystal structure of the perovskite layer on the processes relevant for the operation of a solar cell.

CPP 13.19 Mon 18:30 P1A

Doping design for hole transport materials in perovskite solar cells — •Lorena Perdigón Toro, Christian M. Wolff, Malavika Arvind, and Dieter Neher — University of Potsdam, Soft Matter Physics

In planar perovskite solar cells, the active perovskite semiconductor is usually sandwiched between an organic hole transport material (HTM) and an electron transport material (ETM). The correct choice of these materials has been shown to be crucially important when aiming at high device efficiencies. A promising HTM is the polymeric hole conductor poly(triaryl amine) (PTAA), which given its energetic levels has been shown to be a suitable choice as hole transport and electron-blocking layer. Nonetheless, the relatively low hole mobility of PTAA can be limiting to the performance of the devices, particularly the fill factor and open-circuit voltage. In order to provide sufficient coverage and prevent shunt pathways, thicker hole transport layers (>20 nm) can be efficiently applied provided their mobility can be increased. Therefore, we employ the widely studied electron acceptor F4TCNQ and the strong Lewis acid tris(pentafluorohenyl)borane as dopants for PTAA. Optical spectroscopy of doped solutions and layers insights into the underlying doping mechanisms. The impact of doping on layer morphology is studied by AFM, while the electrical properties are studied with systematic conductivity measurements at different operational conditions (e.g. elevated temperatures). Doped layers are optimized in working devices for highly efficient perovskite solar cells, reaching efficiencies above 18%.

CPP 13.20 Mon 18:30 P1A

Temperature-dependent optical spectra of $(CH_3NH_3)PbBr_3$ single-crystals cleaved in ultrahigh vacuum — •Oskar Schuster[1], Max Wilhelm[1], Daniel Niesner[1], Ievgen Levchuk[2], Andres Osvet[2], Shreetu Shrestha[2], Miroslaw Batentschuk[2], Christoph Brabec[2,3], and Thomas Fauster[1] — [1]Lehrstuhl für Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [2]I-MEET, Department of Materials Science and Engineering, FAU Erlangen-Nürnberg, Martensstr. 7, D-91058 Erlangen, Germany — [3]ZAE Bayern, Haberstr. 2a, D-91058 Erlangen, Germany

Temperature-dependent optical spectroscopy determines basic properties like band gap, exciton binding energy, and direct or indirect character of the gap. Differences have been reported between freshly cleaved crystals compared to as-grown ones or thin films. We present an approach that determines the absorption of cleaved crystals from measured one-photon and two-photon induced photoluminescence spectra. The extracted low-temperature band gap and exciton binding energy of 22 meV are in excellent agreement with the ones determined from other techniques. The direct band gap increases with temperature at < 200 K, and decreases at higher temperature. The behavior is well described by the Bose-Einstein model. The associated exciton binding energy decreases for temperatures > 200 K. We find a second transition 60 meV (90 meV) below the direct gap in the orthorhombic (tetragonal) phase, consistent with a slightly indirect gap. Emission from this transition is significantly reduced after exposing the crystals to air.

CPP 13.21 Mon 18:30 P1A

Photoinduced Charge Generation and Dynamics in Mixed Formamidinium Methylammonium Lead Halide Perovskite Thin Films as Observed by fs Transient Absorption Spectroscopy — •Jonas Horn[1,2,3], Iulia Minda[2], Heinrich Schwoerer[2], and Derck Schlettwein[1,3] — [1]Justus-Liebig-University Giessen, Institute of Applied Physics — [2]Stellenbosch University, Laser Research Institute, South Africa — [3]Justus-Liebig-University Giessen, Laboratory for Materials Science

Hybrid organic inorganic perovskite materials, in particular $FA_{1-x}MA_xPbI_{3-y}Br_y$ using formamidinium and methylammonium cations, are of great interest not only due to the rapid increase in power conversion efficiencies when applied in photovoltaic devices but also due to their astonishing optoelectronic properties. By means of transient absorption spectroscopy in the visible and near infrared spectral regions, temporal evolution of the population and depopulation of various electronic states and their associated spectral signatures was monitored. The detailed interpretation of the results leads to a consistent charge dynamic model of the initial photo-processes. Upon photoexcitation with 3.2 eV photon energy, hot electrons and holes are generated in the lowest conduction band and second highest valence band and relax to the band edges with a time constant of approximately 500 fs. Subsequently recombination, occurring on gradually faster time scales for hot versus cold electrons was shown and assigned to Auger- and bimolecular recombination.

CPP 13.22 Mon 18:30 P1A

Dye-Sensitized Solar Cells based on Low-Temperature Electrodeposited ZnO and Co(II/III) Redox Electrolyte — •Raffael Ruess[1,2], Sebastian Haas[1,2], Andreas Ringleb[1,2], and Derck Schlettwein[1,2] — [1]Justus-Liebig-University Giessen, Institute of Applied Physics — [2]Justus-Liebig-University Giessen, Laboratory for Materials Science (LaMa)

Emerging photovoltaics, such as dye-sensitized solar cells (DSSCs), have received great interest in the recent years because of quite high record efficiencies (<14.3%) and low energy payback times. The present work is focused on DSSCs based on electrodeposited, porous zinc oxide which allows low preparation temperatures to further reduce energy consumption of cell production and allows the preparation on flexible polymer substrates. To reduce voltage loss in the cell and thus improve the power conversion efficiency, the commonly used I^-/I_3^- redox electrolyte in these DSSCs is replaced by a $Co(II/III)$ redox couple. Recombination, electrolyte diffusion and electron transport in the DSSC devices are studied by impedance spectroscopy, intensity modulated photocurrent and photovoltage spectroscopy and charge extraction techniques. It was found that the interaction of the cobalt redox mediator with zinc oxide at the interface lowers the conduction band position of ZnO and, thus, leads to a lower open-circuit photovoltage. However, efficient dye regeneration can be achieved due to sufficient mass transport through the nanoporous system resulting in high photon-to-electron conversion efficiencies.

CPP 13.23 Mon 18:30 P1A

Temperature and illumination intensity dependent photoluminescence of methylammonium lead iodide perovskites — •Fabian Meier, Sebastian Reichert, Seth Niklas Schumann, Alexander Wagenpfahl, and Carsten Deibel — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

Understanding recombination mechanisms of electrical charge carriers is of tremendous importance for understanding the extraordinary power conversion efficiencies, which increased from 4 % up to 21 %. We investigate thin films of methylammionium lead iodide perovskite on top of PEDOT:PSS layer and an ITO layer in terms of their stoichiometric ratio of methylammonium iodide and lead iodide. By confocal photoluminescence measurements we determine direct recombination of electric charges as function of time and spatial location. We discuss our results in terms of illumination intensity as well as temperature dependence and compare it to the energetically resolved emission spectra. We discuss recombination by tail states, also visible in EQE spectra, in view of the performance of solar cells based on the investigated perovskite layers.

CPP 13.24 Mon 18:30 P1A

Stability and Performance of ZnO-based Dye-Sensitized Solar Cells in Contact to a Co(II/III) Redox Electrolyte — •Sebastian Haas[1,2], Raffael Ruess[1,2], and Derck Schlettwein[1,2] — [1]Justus-Liebig-University Giessen, Institute of Applied Physics — [2]Justus-Liebig-University Giessen, Laboratory for Materials Science (LaMa)

The use of $Co(II/III)$ electrolytes instead of the commonly used I^-/I_3^- redox electrolyte represents an attractive way to increase the efficiency of dye-sensitized solar cells (DSSCs). By this approach, attractive efficiencies of up to 14.3 % were reached for TiO_2-based cells. The present work is focused on DSSCs based on low temperature electrodeposited porous zinc oxide, to decrease further the already attractive energy payback time of DSSCs and allow preparation on temperature-sensitive substrates, e.g. polymer foils. Dye stability, electrolyte diffusion and recombination in the DSSC devices are studied by UV-Vis-spectroscopy, impedance spectroscopy and photocurrent-transients. It was found that the dyes $D149$ and $DN216$ are not stable at the ZnO surface in the presence of the $Co(II/III)$ redox couple. Furthermore, a small influence of a hindered diffusion in the DSSCs based on $Co(II/III)$ redox couple compared with DSSCs based on I^-/I_3^- redox electrolyte was observed.

CPP 13.25 Mon 18:30 P1A

Temperature-dependent transient photocurrent measurements on organic-inorganic halide perovskite solar cells — •Ina Kelz[1], Nico Weber[1], Fabian Ruf[1], Tobias Abzieher[2], Nadja Giesbrecht[3], Meltem F. Aygüler[3], Pablo Docampo[3], Heinz Kalt[1], and Michael Hetterich[1,2] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Light Technology Institute (LTI), Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [3]Department of Chemistry, Ludwig-Maximilians-Universität München (LMU), 81377 Munich, Germany

Organic-inorganic halide perovskites as absorber material in solar cells show high power conversion efficiencies exceeding 20%. This is due to their promising properties such as a strong absorption coefficient and a low non-radiative carrier recombination. Additionally fabrication by low-cost production methods is possible. However, basic material properties of perovskite solar cells are not fully understood yet.

In order to gain a deeper insight into the electro-optic material properties temperature-dependent j-V-characteristics are measured. Organic-inorganic halide perovskites exhibit scan rate-dependent hysteresis effects which vary with various parameters such as illumination, bias voltage or temperature. Temperature dependent photocurrent transients show two regimes with different time constants, a fast component with a multi-exponential behaviour and a slow component which can be described by a single exponential function. The time constant of the slow component decreases for increasing temperature.

CPP 13.26 Mon 18:30 P1A

High Energy Resolution Fluorescence Detected X-ray Absorption Spectroscopy on Lead Halide Perovskite Precursors — •Pascal Becker[1,2], Justus Just[1], Charles J. Hages[1], Oliver Müller[2], and Thomas Unold[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Germany — [2]Bergische Universität Wuppertal, Germany

Perovskites as photon absorbers in thin film solar cells have drawn immense attention resulting in a rapid rise in the achieved power conversion efficiencies exceeding 20 % within a few years. Despite the intensive research in this field little is known about the formation process of these perovskite thin films on an atomic level. X-Ray Absorption Spectroscopy (XAS) is a well suited method to investigate electronic and structural properties of thin film materials. Also, residual precursor phases can be identified by this method even when X-Ray Diffraction (XRD) fails to detect. By using high quality and high resolution reference spectra in a linear combination analysis the amount of these secondary phases can be quantified.

Therefore High Energy Resolution Fluorescence detected XAS (HERFD-XAS) measurements were performed on PbI_2, $PbBr_2$, $PbCl_2$ as well as $NH_3CH_3PbI_xCl_{3-x}$ at the *Pb-*L_2 edge. The data reveal a clear fine structure in near edge region as opposed to data from total yield fluorescence detected spectra.

CPP 13.27 Mon 18:30 P1A

Capacitance spectroscopy on perovskite solar cells and MIS devices — •David Diering[1,2], Christian M. Wolff[2], Charles J. Hages[1], Thomas Unold[1], and Dieter Neher[2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany

Hybrid organic-inorganic Perovskites are recently under strong focus for their tremendous rise in efficiency up to 21%. However, it is not fully understood why this class of material shows such a high performance. Capacitance spectroscopy is a powerful method to investigate defects which give rise to recombination processes and therefore influence the solar cell output.

By performing capacitance-voltage and admittance measurements on mixed perovskite $\{\mathrm{Cs/FA/MA}\}\mathrm{PbI}_{(3-x)}\mathrm{Br}_x$ solar cells and metal-insulator-semiconductor(MIS) devices we are able to get information not only about defects but other important material properties such as the dielectric constant, charge carrier type and concentration. The data supports the previous theory of slight n-type to intrinsic behaviour. Further on, evidence for a deep defect level is found.

CPP 13.28 Mon 18:30 P1A

Origin and Location of Trap States in Perovskite Films — •Tobias Seewald[1], Carola Ebenhoch[1], Philipp Ehrenreich[1], Rebecca Milot[2], Susanne Birkhold[1], Laura Herz[2], and Lukas Schmidt-Mende[1] — [1]Department of Physics, University of Konstanz, POB M 680, Konstanz 78457, Germany — [2]University of Oxford, Clarendon Laboratory, Parks Road, Oxford OX1 3PU, UK

Lead halide perovskites have experienced tremendous research interest within the last years. High power conversion efficiencies in combination with the ability of crystal formation during a solution casting process make this material class very attractive for photovoltaic application. For efficient charge carrier generation, it is essential to minimize non-radiative recombination that can be initiated by energetic trap states. For this purpose, we have studied polycrystalline methylammonium lead iodide perovskite films with varying crystal sizes. Morphology and crystallinity have been modified by means of methylamine gas induced defect healing. Time-resolved photoluminescence as well as pump-probe spectroscopy have been applied in order to relate trap state distribution with crystal sizes and grain boundaries. In this study we can demonstrate the importance of large crystal grains, which allow for high carrier mobilities and reduced non-radiative losses that are crucial for efficient solar cell devices.

CPP 13.29 Mon 18:30 P1A

Vacuum chamber for in-operando grazing-incidence X-ray scattering experiments on novel thin-film solar cells — •Bernhard Kalis, Johannes Schlipf und Peter Müller-Buschbaum — TU München,Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

In the past few years hybrid perovskite solar cells have reached power conversion efficiencies of about 20%. Alternatively, organic and other types of hybrid solar cells offer potentially cheap energy supply. The photovoltaic performance of these novel solar cell materials seems to be directly linked to the morphology of the solar cell film. To understand these connections between structural changes of the absorber material due to the influences of temperature and humidity in addition to the aging of the solar cell we use the grazing-incidence small and wide angle X-ray scattering (GISAXS/GIWAXS) method during operation [1]. To fulfil and control all these environmental influences, a newly designed vacuum chamber comes to action that consists of several modules to provide multi-functionality. This Chamber has also the ability to be pre calibrated in order to minimize the expenditure of time during a beam time at a synchrotron such as the ELETTRA in Trieste, Italy or the DESY in Hamburg, Germany.

[1] C. J. Schaffer, C. M. Palumbiny, M. A. Niedermeier, C. Jendrzejewski, G. Santoro, S. V. Roth, P. Müller-Buschbaum, Advanced Functional Materials 2013, 25, 6760.

CPP 13.30 Mon 18:30 P1A

Spectroscopic investigation of trap states related to loss mechanisms in hybrid perovskite solar cells — •Sebastian Reichert, Fabian Meier, Alexander Wagenpfahl, and Carsten Deibel — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

Due to excellent electrical and optical properties of perovskite films for solar cell applications the pace of improvement related to power conversion efficiency and morphological optimisation has been unprecedented. The efficiency of methyl ammonium lead iodide (MAPI) solar cells is limited by the loss of charge carriers which is occurring within the active layer. Choosing a suitable model for those recombination mechanisms is still difficult, also due to the influence of the neighbouring transport or contact layers. We present photoluminescence transients of various MAPI thin films and compare these measurements to theoretical predictions by the charge carrier continuity equation for different recombination models. Depending on the processing conditions, the results indicate recombination assisted by tail states. The energetic trap distribution is quantified by thermally stimulated current measurements. We discuss the dominant recombination process in the examined MAPI films.

CPP 14: Poster: Bioinspired Functional Materials

Time: Monday 18:30–21:00 Location: P1C

CPP 14.1 Mon 18:30 P1C

Rethinking superhydrophobicity — •Schellenberger Frank, Encinas Noemí, Vollmer Doris, and Butt Hans-Jürgen — Max Planck Institute for Polymer Research, Mainz, Germany

To a certain degree, it is possible to control the macroscopic wetting properties of a surface by its nano- and microstructure. In particular, super liquid-repellant-surfaces have received interest due to their many potential applications, such as anti-fouling for for example. Super liquid-repellency can be achieved by nano- and microstructuring a low energy surface in a way, that the structure can entrap air underneath the liquid. The common criteria for super liquid-repellency are a high apparent advancing contact angle and a low contact angle hysteresis. For a better understanding of how a drop advances and recedes on such a structured surface, we imaged the motion of a water drop on a superhydrophobic array of micropillars by laser scanning confocal microscopy (LSCM). With LSCM, we imaged an advancing water front on a superhydrophobic surface at a resolution of 1 *m. The results give a qualitatively new picture of how water advances on the microscopic scale. We demonstrate that in contrast to traditional goniometer measurements, the advancing contact angle is close to 180° or even higher. In contrast, the apparent receding contact angle is determined by the strength of pinning. We propose that the apparent receding contact angle should be used for characterizing super liquid-repellent surfaces [1,2].

[1]F. Schellenberger et al., Phys. Rev. Lett. 116, 096101 (2016) [2]P. Ball, Nature Materials 15, 376 (2016)

CPP 14.2 Mon 18:30 P1C

3D depth profiles of tip–sample interaction on type I collagen fibrils in humid air — •Robert Magerle[1], Manuel R. Uhlig[1], Diana Voigt[1], Martin Dehnert[1], and Anke Bernstein[2] — [1]Fakultät für Naturwissenschaften, Technische Universität Chemnitz — [2]Orthopädie und Traumatologie, Universitätsklinikum Freiburg

The water content and intermolecular crosslinks between collagen fibrils are important factors that determine the mechanical properties of type I collagen fibrils. With atomic force microscopy (AFM) we study reconstituted type I collagen fibrils (without crosslinks) and native fibrils from sheep tendon (with crosslinks). The water content in the fibrils is controlled via the relative humidity of air in the AFM. We measure force–distance (FD) curves and amplitude–phase–distance (APD) curves and reconstruct from this data three-dimensional (3D) depth profiles of the tip–sample interaction. This reveals the contributions of the attractive capillary interaction, the adhesive interaction as well as the repulsive viscoelastic response of the hydrated collagen fibrils. Furthermore, the 3D depth profiles of the tip–sample interaction allow for accurate measurements of the fibrils' shape and the fibrils' swelling behavior with increasing water content. We compare this with the related changes in the fibrils' elastic modulus and discuss the role of water content and intermolecular crosslinks in collagen fibrils.

CPP 14.3 Mon 18:30 P1C

Study of the ion channels insertion in artificial membranes — Marcelo Cisternas[1,2], Vanessa Zepeda[1,2], Maria Jose Retamal[1,2,5], Tomas P. Corrales[3], Nicolas Moraga[1,2], Diego Diaz[1,2], Rodrigo Catalan[1,2], Sebastian Gutierrez[4], Tomas Perez-Acle[4], Patrick Huber[6], and •Ulrich G. Volkmann[1,2] — [1]Instituto de Fisica, P. Univ. Catolica de Chile (UC), Santiago, Chile — [2]CIEN-UC, P. Univ. Católica de Chile (UC), Santiago, Chile — [3]Facultad de Fisica, UTFSM, Valparaiso, Chile — [4]DLab, Fundacion Ciencia y Vida, Santiago, Chile — [5]Facultad de Quimica, P. Univ. Catolica de Chile (UC), Santiago, Chile — [6]Institute of Materials Physics and Technology, TUHH, Hamburg, Germany

The study of artificial membranes is important, because these model-membranes represent the behavior of its biological analogs, with a similar structure, composed of a series of phospholipids and proteins, altering their behavior when exposed to physical and chemical stimulations. This motivates possible applications, for example in the detection and transduction of molecular signals, a very important step in the development of biosensors. In this research we measured the change in the capacitive response of a system, composed by a DPPC bilayer on a thin layer of Chitosan (CH) deposited on a silicon substrate. The system was immersed into a protein solution of gramicidin and the study of the change of the capacitive response confirms the ion channel formation in the bilayer. Acknowledgements: MJR: Fondecyt postdoc 3160803. UGV: Fondecyt 1141105 y CONICYT-PIA ACT 1409. TPC: Fondecyt Iniciación 11160664, MC: CONICYT scolarship.

CPP 14.4 Mon 18:30 P1C

AFM study of evaporated phospholipidic bilayer on thin film chitosan in liquid environment — Rodrigo Catalan[1,3], Maria Jose Retamal[1,2,3], Diego Diaz[1,3], Marcelo Cisternas[1,3], Nicolas Moraga[1,3], Tomas P. Corrales[4], Marco Soto-Arriaza[2], Patrick Huber[5], and •Ulrich G. Volkmann[1,3] — [1]Instituto de Fisica, P. Univ. Catolica de Chile (UC), Santiago, Chile — [2]Facultad de Quimica, P. Univ. Catolica de Chile (UC), Santiago, Chile — [3]CIEN-UC, P. Univ. Catolica de Chile (UC), Santiago, Chile — [4]Facultad de Fisica, UTFSM, Valparaiso, Chile — [5]Institute of Materials Physics and Technology, TUHH, Hamburg, Germany

Self-assembly of artificial biological membranes on solid substrates has gained importance due to the potential applications in the field of BioNanotechnology. Particularly important are phospholipidic membranes, e.g. DPPC, which interact with proteins that regulate the flow of ions across the membrane. In a previous work we have shown that DPPC forms a bilayer on silicon, which can serve for biosensoric applications. We have extended this concept to other phospholipids to explore their interactions with proteins. We present a thermal and morphological study of three phospholipidic thin-films: DODAB, DSPC and DMPC. These films are fabricated by Physical Vapour Deposition (PVD) on silicon and analyzed with Atomic Force Microscopy (AFM) in liquid at various temperatures. We show that these phospholipids do not decompose during PVD. Acknowledgements: MJR: Fondecyt postdoc 3160803. UGV: Fondecyt 1141105 y CONICYT-PIA ACT 1409. TPC: Fondecyt Iniciación 11160664, MC: CONICYT scolarship.

CPP 14.5 Mon 18:30 P1C

Optical characterisation of single setae of the Saharan silver ant — •Bertram Schwind[1], Helge-Otto Fabritius[2], Thorsten Wagner[1], and Xia Wu[1] — [1]Department of Chemistry, University of Paderborn, Warburger Straße 100, 33098 Paderborn, Germany — [2]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

The Saharan silver ant (*Cataglyphis bombycina*) is adapted to extreme hot environmental conditions of the sahara desert [1]. The body of the ant is covered with a dense array of triangular shaped setae [2]. These setae not only reflect the incoming solar radiation by internal total reflection [3], but also enhance radiative cooling [2].

To deepen our understanding on the optical properties of the setae, we measured transmission spectra of single setae by FTIR from the MIR to visible range. Both the chemical composition and the orientation of the setae may have an influence on the shape of the transmission spectra. The absorption bands in the MIR region identify the composition of the setae. The relationship between the structure of the setae (orientation, shape, size, surface morphology) and scattering is investigated by transmission experiments combined with FDTD simulations.

References:

[1] Wehner, R. et al., Nature 357, pp. 586 - 587, 1992; doi: 10.1038/357586a0

[2] Norman, N. S. et al., Science 17 Jul 2015: Vol. 349, Issue 6245, pp. 298-301, doi: 10.1126/science.aab3564

[3] Willot, Q. et al., PLoS ONE 11(4): e0152325. doi:10.1371/journal.pone.0152325

CPP 14.6 Mon 18:30 P1C

Simulation of the Cuticular Photonic Crystals Evolved by the Neotropic Weevil Entimus Imperialis — •Fernando Luis Rodríguez Gallegos[1], Xia Wu[2], and Jens Förstner[1] — [1]Theoretical Electrical Engineering Group, Paderborn University, Germany — [2]Department of Chemistry, Paderborn University, Germany

We analyze the reflectance within the visible spectrum of the photonic crystals found in the scales of the neotropic weevil Entimus Imperialis. Our simulations show that the reflected signal at certain frequencies is cross polarized with respect to the excitation source. We present details of our simulation procedure, explain the underlying mechanism using a reduced equivalent structure and finally show the agreement to our experimental results.

CPP 14.7 Mon 18:30 P1C

Actin stress fiber dynamics under lateral constraint — •Andreas Müller and Tilo Pompe — Universität Leipzig, Institute of Biochemistry, Johannisallee 21-23, 04103 Leipzig

Cells at interfaces experience inhomogeneous mechanical environments, including spatial constraints, even down to 1D confinement, e.g., on single fibers in reconstituted in vitro fibrous scaffolds and also in various tissues in vivo. Previously, we found a bimodal distribution of actin stress fibers in cells under varying lateral constraint, indicated by the distinct formation of exterior and interior stress fibers and their respective spacing. We now investigated the dynamics of stress fiber formation and the correlated cell traction forces.

We use micro-patterned hard substrates and polyacrylamide hydrogels with fibronectin for subsequent culture of cells on stripe-like patterns. Cells are analyzed for several hours using SiR-Actin probes, focusing on actin cytoskeleton pattern, overall cell characteristics, and cell traction forces. We show that the magnitude of traction forces does correlate weakly with lateral constraint while actin cytoskeleton morphology and directionality of traction forces are strongly correlated and governed by the degree of confinement. Furthermore, time resolved actin stress fiber patterns are investigated in relation to cell dynamics.

With our setup, we are able to determine the mechanical and morphological response of cells in spatially constraining environments in a time-resolved manner.

CPP 14.8 Mon 18:30 P1C

Dissipative bio-inspired supramolecular materials — •Marta Tena-Solsona, Benedikt Reiss, and Job Boekhoven — Technische Universität München

Synthetic self-assembled supramolecular materials have enormously developed during last decades. Applications of them are found in healthcare opto-electronics, and a wide range of fields. Although the behavior of these man-made materials is well-known, they are far from competing with biological counterparts. Especially, concerning spatiotemporal control, responsiveness, or adaptivity against external stimuli. The main differences between both type of systems lie in the energy balance. While most artificial assembled materials operate close to the thermodynamic equilibrium, many of the more advanced biological machineries are kinetically governed by self-assembly processes. These processes require a constant input of energy in order to be sustained, and to continuously dissipate energy. This dissipative mode of self-assembly requires specific design rules which are not fully understood in chemically driven man-made materials. Therefore, the design of these dissipative self-assembled systems remains challenging and the number of man-made examples is still limited. Our work focuses on translating the interesting properties biology offers, to the fully synthetic dissipative assemblies. We have designed a chemical reaction network based on small molecules that forms transient, far from-equilibrium materials, by consuming a chemical fuel. The dissipative nature of our system allows us to spatio-temporary control these assemblies which are of colloidal nature or hydrogels.

CPP 15: Poster: Membranes, Biomaterials, Biopolymers

Time: Monday 18:30–21:00 Location: P1C

CPP 15.1 Mon 18:30 P1C

The fluorescence activity of nano-confined dyes — Khalil Alizadeh[2], Seyyed Mahdi Shavakandi[2], Soheil Sharifi[2], Othmar Marti[1], and •Masoud Amirkhani[1] — [1]Universität Ulm Albert-Einstein-Allee 11, 89081 Ulm, Germany — [2]Department of Physics, Faculty of Sciences, Ferdowsi University of Mashhad, Mashhad 91775-1436

Dyes molecules are widely used for imaging, lasing and coloring application thus increasing the photostability and decreasing the quenching rate are very crucial. One way to deal with mentioned problems is embedding dye molecules in the environment, which increase thermal diffusion and also hinder the aggregation. A two-phase medium such as emulsion is an ideal system due to their ability to enhance the solubility and also decrease the dimerization of dye molecules. In this study two Xanthene type dyes (Rhodamine B and Fluorescein sodium salt) are dissolved in a water-in-oil microemulsion. The optical activity of both dyes were examined using their fluorescence and absorption spectrum. Rhodamine B (RhB) florescence activity enhanced in microemulsion solution compare that of in water solution, which can be attributed to a decrease in dimerization. The opposite trend was observed for Fluorescein sodium salt, the difference between the behavior of RhB and FSS is linked to their solubility in water. We additionally, used Lippert-Mataga equation to calculate the change of dipole moments in the ground and exacted states.

CPP 15.2 Mon 18:30 P1C

Surfactant-induced Porous Polymer Film — •Dan Peng[1], Farid Farajollahi[2], Susanne Sihler[3], Ulrich Ziener[3], Othmar Marti[2], and Masoud Amirkhani[2] — [1]Institute of Advanced Materials, Ulm University, Germany — [2]Institute of Experimental Physics, Ulm University, Germany — [3]Institute of Organic Chemistry III, Ulm University, Germany

The basic working mechanism of Breath Figure (BF) method is the condensation of water vapor on the polymer solution during the evaporation of the solvent. Holes structure left on the surface of the polymer film after complete evaporation of solvent and condensed water. BF method is an effective way to prepare ordered-arrangement porous polymer films. The aim of this study is to use a surfactant to produce honeycomb structure of polystyrene films by BF method. Samples cast from polystyrene solution without surfactant in three solvents including chloroform, cyclohexane and toluene show no honeycomb structure. After adding the surfactant into these solutions, the best honeycomb pattern films are achieved from the solution with toluene. The result shows that humidity and evaporation rate effect the structure of pores on the surface.

CPP 15.3 Mon 18:30 P1C

Fabricating Complex Composite Porous Structures — •Yize Shao[1], Susanne Sihler[3], Farid Farajollahi[2], Ulrich Ziener[3], Othmar Marti[2], and Masoud Amirkhani[2] — [1]Institute of Advanced Materials, Ulm University, Germany — [2]Institute of Experimental Physics, Ulm University, Germay — [3]Institute of Organic Chemistry III, Ulm University, Germany

The Breath Figure process is a self-assembly based method for producing honeycomb-structured porous films. In the process, evaporation of the solvent induces cooling of solution surface, which will result in water droplets condensing and arranging into ordered hexagonal structure. In Breath Figure technique,mini-emulsion can be used to help stabilize water droplets condensed on the solution surface. Mini-emulsions are stable systems containing oil, water, and surfactant. It is obtained by a high shear process (ultrasonication technique) resulting in small, homogeneous nanodroplets. In our study, we choose organic solvent such as Chloroform and Toluene as the oil phase to make the mini-emulsion, and we measure the nanodroplets size distribution with the help of dynamic light scattering (DLS). We carry out a series of experiments to explore the different parameters like concentration of polymer, relative humidity and especially the effect of surfactant in the polymer solution on forming ordered hexagonal structures by using the Breath Figure method.

CPP 15.4 Mon 18:30 P1C

Optical studies of thermal properties of materials — •David Schönebeck[1], Jonas Pfeil[1], Anna Sailer[2], Martin Müller[1], Kay-E. Gottschalk[1], and Masoud Amirkhani[1] — [1]Institut für experimentelle Physik, Universität Ulm, D-89069 Ulm — [2]Wissenschaftliche Werkstatt Feinwerktechnik, Universität Ulm, D-89069 Ulm

Polymeric materials adsorb on suspended gold nano particle (GNP) surfaces depending on their solubility behavior in the surrounding medium. GNP have an optical absorption maximum in the visible range. This is where they heat up and can act as point heat sources to their environment. Exploiting this, one can control the solubility of UCST and LCST materials in the vicinity of GNP in the suspension. This has an influence on the hydrodynamic radius of the gold-polymer aggregates. These effects shall be studied by standard DLS investigations, thermal diffusion experiments, and later also fluorescence and fluorescence-correlation spectroscopy. The main goal of this work is to realize an experimental setup that is capable of exciting the GNP and measuring their response at the same time. We use one excitation laser near the absorption maximum and one measurement laser with lower energy pointing at the same or slightly offset position. The centerpiece of the setup is a temperature controlled glass cylinder to house the sample containers at biologically relevant temperatures. Two photon counting detectors, of which one can be rotated around the cylinder by a desired angle, detect the excitation (straight line) and the measurement (rotated) signal from the two light sources separately.

CPP 15.5 Mon 18:30 P1C

A theoretical model of the frame-guided assembly process — •Simon Raschke and Andreas Heuer — Inst. für Phys. Chem., Corrensstr. 28/30, D-48149 Münster

The formation of self assembled structures such as micelles and vesicles has been intensively studied and is well understood. Recent studies [1] use a new approach of vesicle formation by starting with a molecular frame (based, e.g., on DNA) which serves as the basis of new micelles/vesicles. In this way (i) shape and size of the desired micelle/vesicle can be predefined, e.g., by using ellipsoidal rather than spherical molecular frames, and (ii) the ability to generate regularly shaped vesicles can be enhanced.

While the self assembly of micelles/vesicles is relatively well understood, the frame-guided assembly process has not yet been explored in depth from a theoretical perspective. We developed a theoretical model of the frame and the amphiphilic molecules which via Monte Carlo simulations can be analysed to obtain information about the driving forces and the kinetic properties of micelle/vesicle formation. Via optimized simulation routines very large systems can be handled in order to be close to the typical sizes, relevant for the experimental situation.

[1] Dong, Y., Yang, Z. & Liu, D. Small 11, 3768*3771 (2015).

CPP 15.6 Mon 18:30 P1C

Investigating structure and water permeability of bilayers containing beta-cyclodextrin using MD simulations — •Alexander Kötter, Djurre Hendrik de Jong, and Andreas Heuer — Institut für Physikalische Chemie, Corrensstraße 28/30, 48149 Münster

Vesicles, based on amphiphilic cyclodextrin derivatives and phospholipids, display an interesting host guest chemistry. We study permeability and structural properties of corresponding bilayers on coarse grained and atomistic level using molecular dynamics simulations. Comparison of atomistic and coarse grained simulation for exemplary systems suggests that the structural properties are essentially preserved in the coarse grained model. Coarse grained simulations indicate, that variations of the cyclodextrin molecules, such as the length of the alkyl chain, or the length of the ethylglycole group have no significant impact on the the structural or dynamic properties of the bilayers. In particular, free energy calculations as well as the analysis of trajectories suggest that the experimentally observed dependence of the water permeability on the alkyl chain length only results from the presence of different phases in this experiment. In contrast, the introduction of phospholipids to the cyclodextrin bilayers seems to impact the microscopic structural properties of these bilayers severly. This might explain the experimentally observed differences in the shape of the pure cyclodextrin vesicles compared to the mixed phospholipid vesicles.

CPP 15.7 Mon 18:30 P1C

Adhesion of deformable fluctuating interfaces by multiple types of functional complexes — •Josip Vlajčević[1] and Ana-Sunčana Smith[1,2] — [1]Rudjer Bošković Institute, Division of Physical Chemistry, Zagreb — [2]PULS Group, Institut für Theoretische Physik, Univesität Erlangen-Nürnberg

We present a model for the adhesion of flexible fluid membranes to a flat substrate by functional molecules (ligand-receptor pairs) which are freely diffusing on the adherent interfaces. In the absence of molecular complexation, the membrane resides close to a flat surface in a nonspecific potential that originates from van der Waals interactions and the steric repulsion associated with thermal fluctuations. Upon molecular complexation, the interface is deformed introducing cooperative effects for further specific molecular binding. While the system containing only one type functional pairs has been intensively studied in the past, the phase behavior and the dynamics of adhesion mediated by multiple functional pairs is poorly understood.

To rectify this issue we construct a Monte Carlo scheme that appropriately accounts for the described adhesion process. We study the organization of functional pairs into domains as a function of the molecular flexibility, length, binding energies and other properties of the system, and find a very rich phase diagram as a function of these parameters. Furthermore, we apply this model to the adhesion of T-lymphocyte cells, by binding of TCR to pMHC and LFA-1 to ICAM-1 proteins, to explain the fundamental processes in the formation of the immune synapse.

CPP 15.8 Mon 18:30 P1C

Effects of microwaves on graphene quantum dots in solution — •Alexandra Steina, Stefan Fasbender, and Thomas Heinzel — Heinrich-Heine-Universität Düsseldorf, IPkM

Fluorescent graphene quantum dots (GQDs) are prepared by the method of Wu et. al [1] via hydrothermal treatment of citric acid and dicyandiamide with subsequent dialysis to obtain a pure GQD solution. The obtained aqueous solution is treated with microwaves for various times and the effect on the chemical composition of the GQDs is studied with XPS. Fluorescence spectroscopy and UV-vis spectroscopy are used to determine the optical properties of the GQDs.

[1] Wu et al., Nanoscale, 2014, 6, 3868

CPP 15.9 Mon 18:30 P1C

Tight-Binding Simulation of Graphene Quantum Dots — •Christian Wimmenauer and Thomas Heinzel — Solid State Physics Laboratory (IPkM), Heinrich-Heine-Universität Düsseldorf

Graphene quantum dots (GQD) are simulated with an tight binding approach to obtain a better understanding of recent experimental findings regarding the electronic and optical properties of these nanoparticles. The emphasis lies on studying the influence of different edge structures, functional groups and defects on the fluorescence spectra. Using the KWANT software package, hexagonal zigzag edge type, as well as armchair edge type, GQDs have already been modeled. The results are supposed to be used to prepare GQDs with improved optical properties for biological applications.

CPP 15.10 Mon 18:30 P1C

Analysis of orange graphene quantum dots for biological applications — •Lisa Zimmermann[1], Stefan Fasbender[1], Ron-Patrick Cadeddu[2], Rainer Haas[2], and Thomas Heinzel[1] — [1]Heinrich Heine Universität Düsseldorf, IPkM — [2]Universitätsklinikum Düsseldorf, Klinik für Hämatologie

Orange fluorescent graphene quantum dots (GQDs) with an excitation optimum around 500 nm are prepared by thermal decomposition of citric acid and diethylenetriamine slightly modifying the method of Qu et al. [1]. In order to analyse the properties of the particles X-ray photoelectron spectroscopy spectra as well as fluorescence and UV-vis spectra are taken. The latter ones provide the photoluminescence quantum yield of the GQDs. The uptake of GQDs into primary human blood cells is investigated using flow cytometry and visualised via confocal microscopy.

[1] Qu et al., Light: Science & Applications, 2015, 4, e364

CPP 15.11 Mon 18:30 P1C

Polymer chains: how they influence the red blood cell motion — •Carina Bezold, Christian Bächer, and Stephan Gekle — Univesität Bayreuth

A system called glycocalyx covers the luminal surface of blood vessels. The interaction between glycocalyx, represented by polymer chains, and red blood cells and between glycocalyx and the blood flow are examined with the simulation package ESPResSo. Our simulation results show that the velocity of the red blood cell and the effective viscosity of the fluid are altered significantly by the presence of polymer chains.

CPP 15.12 Mon 18:30 P1C

Controlled Assembly of Plasmonic Core/Satellite Nanostructures for Efficient SERS Enhancement — •Roland Höller[1], Izabella Jahn[2], Martin Dulle[3], Dana Cialla-May[2], Martin Mayer[1,5], Stephan Förster[3], Jürgen Popp[2], Munish Chanana[4], Christian Kuttner[1,5], and Andreas Fery[1,5] — [1]Leibniz Institute of Polymer Research, 01069 Dresden, Germany — [2]Leibniz Institute of Photonic Technology, 07745 Jena, Germany — [3]Physical Chemistry I, University of Bayreuth, 95440 Bayreuth, Germany — [4]Institute of Building Materials, ETH Zürich, 8093 Zürich, Switzerland — [5]Cluster of Excellence Centre for Advancing Electronics Dresden (cfaed) and Technische Universität Dresden, 01062 Dresden, Germany

We present a novel protein-assisted self-assembly route of small spherical gold or silver NPs (as satellites) with a hydrophilic protein corona onto larger gold NPs (as cores) into three-dimensional nanoassemblies with core/satellite architecture in dispersion. Their interparticular gaps represent hot spots for surface-enhanced Raman scattering (SERS) detection. The highly modular bottom-up fabrication of homo- and heterometallic core/satellite combinations allows for tailored plasmonics. A precise characterization of the morphology in dispersion was achieved using small-angle X-ray scattering (SAXS). By combining the results from SAXS, UV/Vis spectroscopy, and electromagnetic simulations we were able to correlate the structural parameters with the plasmonic coupling within the core/satellite nanoclusters.

[1] Höller, R.P.M. et al., ACS Nano 2016, 10, 5740-5750.

CPP 15.13 Mon 18:30 P1C

The Dielectric Permittivity of Protein Solutions — •Susanne Liese and Roland R. Netz — Department of Physics, Free University Berlin, Arnimallee 14, 14195 Berlin, Germany

Electrostatic interactions are essential to understand the conformation and function of proteins. For a quantitative understanding of electrostatics of biological systems, for instance to describe the internal electric field of transmembrane proteins, the dielectric permittivity of proteins has to be known. We here present molecular dynamic simulations of protein solutions, which especially allow us to take the interaction of the protein and the hydration water into account. By studying the dielectric permittivity in dependence of the protein concentration, we can extrapolate our results to the limit of a pure protein and disentangle water and protein contributions to the electrostatic interaction.

CPP 16: Poster: Modelling and Simulation of Soft Matter

Time: Monday 18:30–21:00 Location: P1C

CPP 16.1 Mon 18:30 P1C

Kinetic properties of liquid crystals from coarse-grained and atomistic molecular dynamics simulations — •Svenja Wörner, Joseph Rudzinski, Kurt Kremer, and Tristan Bereau — Max-Planck-Institut für Polymerforschung, Mainz, Germany

Liquid crystals display liquid-like behavior while maintaining a long-range crystalline order, giving rise to unique material properties. To understand macroscopic processes, e.g. phase transitions, large systems need to be studied on time scales not accessible by atomistic models. Coarse grained models make these sizes and time scales accessible.

In this work we investigate the liquid crystal mesogen 8AB8, containing a stiff, photoisomerizable azobenzene core with flexible alkyl tails. Mukherjee et al. have previously developed a coarse-grained model of 8AB8, which displays the correct thermodynamic and structural properties. Not only is it able to form a smectic phase, the model also reproduces the transition temperature of the disordered to smectic phase transition of the underlying atomistic model. Reducing the degrees of freedom usually leads to a non-trivial modification of the timescales for different processes sampled by the coarse-grained model. Two well-characterized translocation pathways in the smectic A phase are studied in detail, utilizing a Markov state model framework to systematically assess the differences in the transport kinetics between the coarse-grained and atomistic models. Investigating the precise source of the discrepancies between the two models implicates an approach for reparametrization of the coarse-grained model.

CPP 16.2 Mon 18:30 P1C

Systematic Reduction of Chemical Compound Space using Coarse-Graining and Clustering Algorithms — •Kiran Kanekal, Kurt Kremer, and Tristan Bereau — Max Planck Institute for Polymer Research

The size of chemical compound space is prohibitively large for the fast generation of hypersurfaces that define structure-property relationships, which are necessary for implementing inverse molecular design. In this work, we use a dataset consisting of all small organic molecules with up to 8 heavy atoms (i.e. excluding hydrogen atoms) as an initial proxy for the entire chemical compound space. This relatively small slice of the total space consists of ~100,000 molecules. We demonstrate a reduction of this space in two steps. First, we apply the AutoMartini algorithm developed by Bereau and Kremer to systematically determine a coarse-grained representation for each molecule in the dataset. We subsequently cluster molecules by using similarity measures corresponding to specific chemical and structural descriptors. We then assess the extent to which the initial chemical compound space was reduced and whether the diversity of the space is sufficiently reflected in its coarse-grained counterpart. The resolution of the coarse-grained space can then be tuned either by introducing new bead types or by reducing the number of atoms assigned to a bead. This framework will provide a means for efficient high throughput sampling of chemical compound space (as highlighted by Menichetti and coworkers in their work).

CPP 16.3 Mon 18:30 P1C

Sampling of chemical space via high-throughput molecular dynamics simulations — •Roberto Menichetti, Kurt Kremer, and Tristan Bereau — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

The increasing request for new materials with tunable physical and chemical properties requires a rational optimization of molecular structures. An exhaustive characterization of all compounds is clearly unfeasible in practice, due to the overwhelming size of chemical space. Instead, we introduce a stochastic Monte Carlo importance sampling approach, in which thermodynamic properties are computed, at every step, by means of high-throughput molecular dynamics simulations. Though chemically heterogeneous, the resulting ensemble of molecules optimizes the target property of interest. In this work, we describe our methodology and apply it to the case of the free energy of insertion of a compound in a phospholipid membrane.

CPP 16.4 Mon 18:30 P1C

Dynamics of Seeded Aβ40-Fibril Growth from Atomistic Molecular Dynamics Simulations: Kinetic Trapping and Reduced Water Mobility in the Locking Step — •Nadine Schwierz[1], Christina V. Frost[2], Phillip L. Geissler[1], and Martin Zacharias[2] — [1]Chemistry Department, University of California, Berkeley, California 94720, United States — [2]Physik Department, Technische Universität München, 85748 Garching, Germany

Filamentous β-amyloid aggregates are crucial for the pathology of Alzheimer's disease. Despite the tremendous biomedical importance, the molecular pathway of growth propagation is not completely understood and remains challenging to investigate by simulations due to the long time scales involved. Here, we apply extensive all-atom molecular dynamics simulations in explicit water to obtain free energy profiles and kinetic information from position-dependent diffusion profiles for different Aβ fibril growth processes. Our approach provides insight into the molecular steps and allows close agreement with experimental binding free energies and macroscopic growth rates. Water plays a decisive role, and solvent entropy is identified as the main driving force for assembly. Fibril growth is disfavored energetically due to cancellation of direct peptide-peptide interactions and solvation effects. The kinetics of growth is consistent with the characteristic dock/lock mechanism, and docking is at least 2 orders of magnitude faster. In the locking step, the dynamics is much slower due to kinetically trapped conformations and the reduced mobility of hydration water.

CPP 16.5 Mon 18:30 P1C

DPD study of Polymer Ring Brushes — •Martin Jehser[1,2] and Christos N. Likos[2] — [1]Department of Physical Chemisrty, University of Vienna, Ausrtia — [2]Faculty of Physics, University of Vienna, Ausrtia

Recently, experimental methods have been developed allowing the production of well defined surface-grafted polymer nanoparticle systems without free chain-ends [1], i.e., grafted polymer loops or rings. In the present investigation, equivalent situations are studied making use of computer simulations based on Dissipative Particle Dynamics [2,3] (DPD) a highly efficient, coarse grained, method smoothly covering the range from several nanometers up to the mesoscale region. In order to reproduce the behaviour of adsorbed polymers in addition to the conservative forces an attractive interaction between one (or in case of loops both) chain end(s) and a surface, represented by a soft wall, are introduced as well. Aim of the study is the comparison of properties of loops and rings to those of trails as functions of surface coverage free chain concentration and particle distance.

The results show that with increasing grafting density, loops and rings become more and more rodlike in structure and increase the layer thickness in the same way as linear chains do. A rise in concentration of free polymer chains results into a compression of the brush.

[1] R. Rotzoll, P. Vana, Journal of Polymer Science Part A: Polymer Chemistry 46, 7656 (2008) [2] R.D. Groot, P.B. Warren, J. Chem. Phys. 107, 4423 (1997) [3] M.M. Nardai, G. Zifferer, J. Chem. Phys. 131, 124903 (2009)

CPP 16.6 Mon 18:30 P1C

Application of molecular dynamics simulations to the elasto plastic model — •Lawrence Smith and Andreas Heuer — Institute of Physical Chemistry, WWU Münster, Germany

We are studying the rheology of amorphous solids through the coupling of minimal systems in the athermal limit. This ansatz is based on an exisiting elasto plastic model [1] while reducing the abstraction by using real molecular dynamics (MD) simulations as microscopic states.

For the microscopic systems, a well investigated Lennard-Jones model of N=130 particles is employed. This size approximately corresponds to the number of particles known to participate in a plastic rearrangement. Multiple instances of this system are arranged on a lattice and interact during plastic events by distributing shear stresses. This distribution follows the standard elastic propagator $\cos(4\theta)/r^2$.

We study the relevant ingredients of this model to identify plasticity during running MD simulations. Of key interest are the impact of the coupling on stress drop distributions and spatial correlations of plasticity as well as on the behaviour of the system during row.

[1] Nicolas, A., Martens, K. and Barrat, J. L. *EPL* **107,** 44003 (2014)

CPP 17: Poster: Polymer Networks and Dynamics

Time: Monday 18:30–21:00 Location: P1C

CPP 17.1 Mon 18:30 P1C

Shear deformation of model networks: A Monte-Carlo-Study — •Toni Müller[1,2], Michael Lang[1], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden — [2]Technische Universität Dresden

Using the bond-fluctuation model, we compare the elastic properties of end-linked model networks with model systems where either entanglements or both entanglements and excluded volume were switched off in the computer simulation. In our simulations we apply a shear-stress to the periodic simulation box and calculate the deformation in equilibrium. The goal of this study is to consider the contribution of connectivity and of topological constraints to the shear modulus separately. We expect further insight into the influence of network defects and the impact of excluded volume on the elasticity. As a result we can make an reasonable estimate for the entanglement degree of polymerization.

CPP 17.2 Mon 18:30 P1C

Theoretical and experimental investigations of sealing systems — •Felix Senf[1], Robin Fonk[2], Sean Schneeweiss[2], Ulrich Simon[2], and Othmar Marti[1] — [1]Institut für Experimentelle Physik, Ulm — [2]Ulmer Zentrum für wissenschaftliches Rechnen, Ulm

The following investigation is about leak tightness between surface structures as well as material data to describe critical leakage systems. In technical applications the sealing of hardware components is described with leakage rates based on different boundaries of the system. In general, physical rules state that an absolutely sealed system is not possible. Different parameters like materials, surface structures, roughness parameters, closing forces and not least the design of the sealing system influence the function of the sealing joint. Engineer standards to describe the surface influence of sealing are only based on roughness parameters of the hardware surface. They don't consider that roughness parameters are only statistical parameters with limited information to the real sealing behavior of the joint. Therefore the real systems can show high tolerances in sealing limits. The research program is about understanding the alignment between elastomers and metal surface structures and the resulting open volumes. The theory of contact problems, FEA simulation tasks and compression experiments help us to describe this alignment. An experimental set up for leakage measurements and the combination with CFD simulation are the main part to understand the leakage nature more detailed. Out of this toolbox we want to create a new practical understanding on how sealing works.

CPP 17.3 Mon 18:30 P1C

Low-frequency dynamics of anisotropic magneto-sensitive elastomers — Dmytro Ivaneyko, •Vladimir Toshchevikov, and Marina Saphiannikova — Leibniz-Institut für Polymerforschung Dresden

The low-frequency dynamics of magneto-sensitive elastomers (MSEs) with isotropic, chain-like and plane-like distributions of magnetic particles is studied under a uniform magnetic field H. A coarse-grained network model is used, in which the magnetic particles are positioned on the sites of a tetragonal lattice [1]. The lattice anisotropy is defined by the ratio α of average distances between neighboring particles along and perpendicular to the symmetry axis of an MSE. In our calculations we take into account the influence of the elastic network and magnetic interactions between the particles under the magnetic field. It is shown that the relaxation spectrum of MSE depends on α. The dynamic storage G' and loss G" moduli are calculated for three different geometries of application of the oscillating shear strain with respect to the symmetry axis of MSE, coinciding with the direction of H. The application of the magnetic field leads to a strong anisotropy of G' and G" moduli. Moreover, G' and G" can change up to several orders of magnitude in agreement with recent experiments.

[1] Ivaneyko D. et al., Soft Matter, 2015, 11, 7627-7638; Ivaneyko D. et al., Soft Matter, 2016, submitted.

CPP 17.4 Mon 18:30 P1C

FORC measurements in magnetic elastomers using molecular dynamic simulations — •Alla Dobroserdova[1], Pedro Antonio Sanchez Romero[2], Julia Linke[3], Thomas Gundermann[3], Sofia Kantorovich[1,2], and Stefan Odenbach[3] — [1]Ural Federal University, Lenin av. 51, 620000, Ekaterinburg, Russia — [2]University of Vienna, Sensengasse 8, 1090, Vienna, Austria — [3]Dresden University of Technology, Helmholtzstr. 10, 01069 Dresden, Germany

Magnetic elastomers consists of magnetic particles distributed in a nonmagnetic elastic matrix. We use the FORC (first-order reversal curves) diagrams [C. R. Pike et al., J. Appl. Phys. 85, 6660 (1999)] to study how the matrix influences the internal magnetic interactions. Following the protocol of experimental measurements, we use Molecular Dynamics Simulations to model the system. We consider two different systems. In the first one, fixed nonmagnetic particles are connected with dipolar ones by springs to mimic magneto elastic coupling. In the second system, dipolar particles are replaced by magnetisable colloids. The first step is to get the main hysteresis loop of this system (changing the direction and intensity of an external magnetic field). The second part of the study includes the computer simulations to obtain the first-order reversal curves. In the result, we have the FORC diagrams in dependence of the coercive and the reversal fields. The research was supported by the RFBR Grant 16-52-12008 and the DFG Grant Od18/24-1 within the German-Russian Research Collaboration PAK907.

CPP 17.5 Mon 18:30 P1C

Nitrogen-doped graphene as an alternative to eco-toxic zinc oxide in rubbers — Yulia Glebova[1,2], •Nikolai Severin[1], Vladimir Shershnev[2], and Jürgen P. Rabe[1] — [1]Department of Physics & IRIS Adlershof, Humboldt-Universität zu Berlin, Germany — [2]Moscow State University of Fine Chemical Technologies, Russia

Zinc Oxide (ZnO) is an essential ingredient of industrial rubber production, it regulates the vulcanization onset, accelerates vulcanization kinetics, and improves the mechanical properties of rubber. However, environmental pollution with ZnO is of concern, since it is recognized to be significantly eco-toxic, and it might have also adverse effects on human health. One of the major sources of ZnO environmental pollution is rubber items, in particular tires. Nitrogen (N-) doped graphene is a promising next generation catalyst comparable in its efficiency to platinum. We show that replacement of 3 phr (weight parts per hundred weight parts of polymer) of ZnO by just 0.1 phr of N-doped graphene in styrene-butadiene rubber reduces the vulcanization onset time by more than a factor of two while keeping the fast vulcanization kinetics and enhancing the tensile strength as compared to the rubber with just ZnO. Shorter vulcanization time implies saving energy, which together with the non-toxicity of N-graphene should make the resulting rubbers substantially more environmentally friendly.

CPP 17.6 Mon 18:30 P1C

Topological interactions in polymers under shear — Maciej Kawecki[1], Franz Adlmann[1], Philipp Gutfreund[2], Sudipta Gupta[3], Peter Falus[2], David Uhrig[3], and •Max Wolff[1] — [1]Department for Physics and Astronomy, Uppsala Univeristy, Sweden — [2]Institut Laue-Langevin, Grenoble, France — [3]Oak Ridge National Laboratory, Oak Ridge, TN, USA

Since decades topological interactions as described by the reptation theory of DeGennes, Doi and Edwards are among the most successful concepts in physics. The scaling laws and viscoelastic properties in polymers are predicted correctly. However, currently no such generalized theory is available for large deformations, where shear thinning occurs. Even more, until now, no experimental approach allowed to test possible extensions of the reptation theory, such as convective constrain release, which would have the potential to theoretically predict the shear thinning transition. We present a neutron spin echo based method to directly measure and quantify nanoscale dynamics in flowing liquids and we extract the chain dynamics in a polymeric melt beyond the shear thinning transition. Under flow we find an additional relaxation process, which we attribute to shear thinning and which is in line with the theory of convective constrain release.

CPP 17.7 Mon 18:30 P1C

Thermal, collective and self-diffusion of linear and cross-linked PMMA — •Bastian Pur[1], Werner Köhler[1], Martin Schneider[2], Klaus Huber[2], Alexei F. Privalov[3], and Max Schäfer[3] — [1]Physikalisches Institut, Universität Bayreuth, 95440

Bayreuth, Germany — [2]Physikalische Chemie, Universität Paderborn, 33098 Paderborn, Germany — [3]Institut für Festkörperphysik, Technische Universität Darmstadt, 64289 Darmstadt, Germany

Present theories for polymer thermophoresis discuss two theoretical models: draining coil (Rouse) and nondraining coil (Zimm). In order to discriminate between these models we have startet a comparative investigation of linear chain polymers and cross-linked polymers (microgels). The linear polymer samples are poly(methyl-methacrylate) (PMMA) and the microgel samples are PMMA cross-linked with different amounts of ethylenglycole-di-methacrylate (EGMA). In either case toluene is used as solvent. By means of a transient holographic grating technique we obtained the Fickian diffusion coefficient D, the thermal diffusion coefficient D_T and the Soret coefficient S_T as functions of the polymer concentration c. Using NMR diffusometry in ultrahigh static magnetic field gradients we have determined the self-diffusion coefficient D_s. For c $\rightarrow$ 0 the thermophoretic mobilities of the linear polymers and the microgels with 3.5% EGMA are identical within experimental accuracy. The concentration dependence of D_T is, however, different, with a more pronounced slowing down of the microgel. Against our assumption, D_s of the microgel shows an even stronger concentration dependence, indicating different fricition mechanisms.

CPP 17.8 Mon 18:30 P1C

Influence of Structure on the Slip Boundary Condition of Polymeric Liquids: Experiments and MD-Simulations — •Mischa Klos[1], Laurent Joly[2], Sebastian Backes[1], Sascha Thieltges[1], Kirstin Kochems[1], and Karin Jacobs[1] — [1]Saarland University, Dept. of Experimental Physics, D-66041 Saarbruecken — [2]Univ Lyon 1, Inst Lumiere Mat, 43 Blvd 11 Novembre 1918, F-69622 Villeurbanne

In the classic case of a liquid running through a pipe, the flow velocity is usually the fastest in the center and decreases towards the walls. On small scales, the importance of this interface grows. In fact, on a microscale and under certain conditions, a liquid can reach a velocity at the interface (slippage). We study slippage of thin polymer films on two differently ordered types of self-assembled silane monolayers (SAM), as well as on an amorphous PTFE surface. The influence of the liquid*s and substrate*s structure on slippage is examined in dewetting experiments of polymers with various side groups. It turns out that PS on a SAM of relatively low degree of order shows an usual high slip length, whereas slip is reduced if PMMA or polyvinylpyridine (PVP) is used instead of PS. The specific kind of order plays a major role. Insights on the structure are gained with the help of X-ray reflectometry and MD-simulations. MD-simulations could mimic experimentally observed structural and dynamical data and enabled new insights to the mechanisms at the solid/liquid interface.

CPP 17.9 Mon 18:30 P1C

Non-monotonic effect of small molecules on the glass transition temperature of entangled polymers — •Elias Mahmoudinezhad and Fathollah Varnik — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), IC 02-753, Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum, Germany

Using molecular dynamics simulations, we aim to study how the presence of small particles within a polymer melt affects its glass transition temperature, T_g. In this study, T_g is determined via standard cooling simulations from the liquid state to the glassy phase. We use a variant of a well-established fully flexible polymer model, first proposed by Kremer and Grest [1], extended by the attractive part of the Lennard-Jones interactions. The chain length, N_p is chosen larger than the entanglement length of the model (N_p=64 > N_e~=32, see Refs. [1, 2]). The size of small particles is smaller than the monomer diameter and is varied in a wide range. It is found that the size of small particles plays a crucial role for the T_g of the investigated polymer-particle mixture. Importantly, the glass transition temperature of the system changes in a non-monotonic way with the size of small particles. Our results are in qualitative agreement with experiments on polymers. The present observations can also be rationalized in terms of a recent mode coupling theory for binary mixtures [3], thus highlighting the generic character of the observed non-monotonic behavior [4].

CPP 17.10 Mon 18:30 P1C

Simulation study of a PMMA chain with azobenzene side groups near a silica surface — •Markus Koch[1,2] and Olga Guskova[1,3] — [1]Leibniz-Institute of Polymer Research Dresden, Hohe Str. 6, 01069 Dresden — [2]Institute of Theoretical Physics, Technische Universität Dresden, 01069 Dresden — [3]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden

In recent years, azobenzene-containing hybrid materials have been of high scientific interest due to their strong responses under external illumination with light. The most striking feature of azobenzenes (azo) is a fully reversible photoisomerization between its trans- and cis-states. When azo-groups are coupled to polymeric systems, this isomerization reaction induces conformational changes and stresses on larger length scales. This makes such materials very promising for applications in nano- and microtechnology.

Here, we present the results of a simulation investigation approach to model the systems with Ångström resolution. Our study combines DFT calculations for a comprehensive analysis of the electronic and optical properties of specific azo-compounds with all-atom MD simulations to investigate the dynamical behavior of polymers with covalently attached azo side-groups. In particular, we present the dynamic behavior of a PMMA chain with covalently attached side groups of Disperse Red-1 acrylate, which is grafted to a silica substrate.

We highly appreciate the financial support from DFG (project GU 1510/3-1).

CPP 18: Poster: Colloids and Complex Fluids

Time: Monday 18:30–21:00 Location: P1C

CPP 18.1 Mon 18:30 P1C

Entropic interactions between dendrimers and linear chains in solution — •Martin Wengenmayr[1,2], Ron Dockhorn[1,2], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Germany — [2]Technische Universität Dresden, Germany

Entropic interactions between soft objects are not fully understood. In particular, branched polymers immersed in a melt of linear chains might segregate even without repulsive interactions between the polymers. To study these effecs for a well defined system, we investigate the conformational properties of dendrimers immersed in dilute to highly concentrated polymer solutions of linear chains. A mean-field theory and large scale computer simulations utilizing the bond fluctuation model are applied to identify the solution properties and repulsive interactions between solvent and dendrimer. The free energy landscape is evaluated applying the Umbrella Monte Carlo sampling methode. Our study shows that the interactions between linear polymer solution and dendrimer depend essentially on the dendrimer generation and on the polymer concentration.

CPP 18.2 Mon 18:30 P1C

DCMIX3b: First results from microgravity experiments on the ISS — •Thomas Triller and Werner Köhler — Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany

DCMIX3b is the most recent iteration of a measurement campaign, which aims to gather a reliable data basis for diffusive transport coefficients of different ternary liquid mixtures in the microgravity environment of the ISS. Special focus of these measurements is the Soret effect, a diffusive demixing driven by a temperature gradient. To get reliable reference data for ground measurements, several international research teams cooperate in the DCMIX project under the auspices of ESA and Roscosmos. DCMIX3 shall provide data for aqueous systems, containing mixtures of water / ethanol / triethylene-glycol. All samples are measured via digital optical interferometry (SODI) inside the Microgravity Science Glovebox. After the loss of the first DCMIX3 samples during the explosion of the Cygnus CRS Orb-3 transport in October 2014, measurements had to be deferred for almost two years. In July 2016, the new DCMIX3b samples were successfully delivered to the space station by SpaceX CRS-9. Starting in September 2016, a set of 30 experimental runs with 5 different compositions could be performed until the end of operations in November 2016. Full evaluation can only begin after the hard disks containing the data will be brought back to earth, probably in early 2017. Nevertheless, the available telemetry data gives a good impression of the quality of the data. On our poster, we show a first assessment, explaining the evaluation process, as well as some problems which occurred during operations.

CPP 18.3 Mon 18:30 P1C

Optical contrast factor measurements of ternary mixtures with a multi-wavelength Michelson interferometer — •Marcel Schraml and Werner Köhler — Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany

Non-isothermal diffusion in ternary mixtures is extensively studied both on ground and under microgravity conditions on the Internation Space Station ISS (ESA/Roscosmos, DCMIX3). In most cases are optical, contactless techniques the method of choice. These methods have the disadvantage that the measured data need to be transformed from the refraction index space into the concentration space. Therefor the contrast factor matrix $a_{ij} = \left(\partial n_i/\partial c_j\right)_{p,T,c_{k\neq j}}$ has to be inverted. At least two different wavelengths are necessary to provide sufficient information for ternray mixtures. We have designed a multi-wavelength Michelson-Interferometer to get precise refraction index values over the whole spectral range measured simultaneously with the same specimen. The Michelson interferometer uses optical fibers to couple the four lasers (406nm, 543 nm, 632 nm, 934 nm) into the experimental setup. The number of wavelengths can easily be extended. The geometrical path is varied and the optical path is measured. At the moment there is no commercial setup available. On the poster we will discuss the present state of the instrument, its design and the achievable accuracy.

CPP 18.4 Mon 18:30 P1C

Influence of added crosslinker on the kinetics of LLPS studied by USAXS — •Richard Schäufele[1], Stefano Da Vela[1], Johannes Möller[2], Fajun Zhang[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]ESRF, Grenoble, France

In the presence of trivalent cations, e.g. Y^{3+}, BSA solutions feature a liquid-liquid phase separation (LLPS) with a lower critical solution temperature. During LLPS the dense phase of the system can be brought to a dynamically arrested state before reaching the binodal for temperatures below denaturation.[1] By adding a bifunctional crosslinker, Glutaraldehyde, protein monomers form clusters based on inherently multiple reaction sites. Crosslinker concentration directly impacts size and size distribution of protein clusters, altering the binodal as well as the glass line. In order to understand the influence of oligomerization on the kinetics of LLPS and the arrested state, dense phases with different crosslinker concentrations are studied. The experiments focus on the kinetics during phase separation for different temperature quenches. By using time-resolved ultra small angle X-ray scattering (USAXS) complemented with DLS, the evolution of the characteristic length can be followed through the different stages of the phase separation. Surprisingly, an increasing crosslinker concentration does not display a monotonic trend considering the characteristic length. The latter as well as the behaviour of intensity and arrested state will be discussed with respect to the temporal evolution.
[1] Stefano Da Vela, et al., Soft Matter, 2016, 12, 9334-9341

CPP 18.5 Mon 18:30 P1C

Characterization of Marangoni convections in microchannel structures — •Daniel Zapf, Michael Orlishausen, Lorentz Butzhammer, and Werner Köhler — Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany

We have investigated Marangoni convection at the meniscus formed by a liquid-gas interface in microchannel structures with characteristic length scales of the order of 100 μm. In ethanol-water mixtures Marangoni convection is driven both by temperature and composition gradients, in pure ethanol by temperature gradients alone. The temperature and concentration differences arise instantaneously from inhomogeneous evaporation at the liquid-gas interface but can also be induced and switched by selective laser heating. The resulting flows are visualized by polystyrene tracer particles of 600 nm in diameter under a light microscope. Particle velocities are determined via image correlation techniques. As a function of the meniscus shape, the microchannel geometry and the evaporation rate of the volatile component, either a single or two symmetric convection roles are observed. They come to a sudden halt when the evaporation of the liquid is stopped by an increas of the vapor pressure in the gas phase. Currently we are working on the pressure measurement in the microchannels. Tracer particles are repelled from stream lines that come closer to the meniscus than one particle radius. Surprisingly, this leads to large depletion zones and very efficient particle accumulation inside the vortex. We will present a quantitative analysis of the flow patterns and numerical simulations of the development of the depletion and accumulation zones.

CPP 18.6 Mon 18:30 P1C

Binding probability model for protein cluster formation in aqueous solution — •Michal K. Braun[1], Marco Grimaldo[2], Felix Roosen-Runge[2], Tilo Seydel[2], Fajun Zhang[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]ILL, Grenoble, France

Due to the specific nature of the interactions, in certain cases protein crystallization can be described by a model of globular particles with attractive patches [1]. Clusters of proteins are possible precursors for crystals. We have investigated self-diffusion [2] and collective diffusion [3] of clusters of the model protein bovine serum albumin (BSA) that form in the presence of a trivalent salt (YCl$_3$). The self- and collective diffusion coefficients are obtained from neutron and dynamic light scattering (DLS) data, respectively. We present new DLS data on BSA in the presence of another trivalent salt, namely LaCl$_3$. Our data can be analyzed based on simple Brownian diffusion [2]. The total scattering function S(q, ω) is linked to the model of patchy particles. In this way, the dependence of the binding probability p_b on the salt concentration is obtained. The measured self- and collective diffusion coefficients fall onto separate master curves [2,3], which only depend on the ratio of salt and protein. In the case of self-diffusion a master curve was also found for p_b. From the new collective diffusion data p_b will be extrated analogously and will be compared to p_b from the self-diffusion data.
[1] Roosen-Runge et al., *Sci. Rep.*, **4**, 7016, 2014
[2] Grimaldo et al., *JPCL*, **6**, 2577, 2015
[3] Soraruf et al., *Soft Matter*, **10**, 894, 2014

CPP 18.7 Mon 18:30 P1C

Influence of poly(ethylene glycol) chain length on ionic w/o microemulsions — •Ann-Kathrin Grefe, Alexander Matt, and Bernd Stühn — Institut für Festkörperphysik, Technische Universität Darmstadt, D-64289 Darmstadt, Germany

Microemulsions are thermodynamically stable mixtures of a hydrophilic and a hydrophobic component, stabilized by surfactants. There have been extensive studies in order to determine how the presence of foreign molecules influences the behaviour of a microemulsion.

We study the droplet phase of water-in-oil microemulsions containing the anionic surfactant dioctyl sulfosuccinate (AOT). The droplets are loaded with the water soluble polymer poly(ethylene glycol), which is expected to dissolve in the water droplets and shows attractive interactions with the surfactant shell [1]. We investigate different molecular weights of PEG ranging from 200 g/mol to 12000 g/mol. In doing so, we are able to differentiate between the influence of chain length and number of hydroxy groups. The influence of the polymer on percolation and phase separation temperature T_P and T_C is examined. To determine T_P and T_C we use dielectric spectroscopy at a frequency of 10 kHz utilizing the steep increase in conductivity as the percolation temperature is approached. In addition, the temperature dependent radii of the water droplets are investigated via small angle x-ray scattering, using the pronounced electron density contrast of the surfactant shell. By combining the results we can calculate the bending modulus of the surfactant shell.

[1] R. Wipf et al., Colloid Polym Sci 288, 589-601 (2010)

CPP 18.8 Mon 18:30 P1C

Investigation of dynamical properties of a simple patchy particle model by Monte Carlo simulations — •Marc Habiger, Johannes Bleibel, and Martin Oettel — Institut für Angewandte Physik, Universität Tübingen, Deutschland

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 like interactions, additionally the colloid-bond interaction contains a short-range, isotropic attraction. The maximum number of bonds on a colloid can be tuned via the repulsion between bonds and is set to four. 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 (dynamic) Monte Carlo simulations.

We have examined the equation of state, and further we investigate the self and distinct part of the dynamical structure factor and the intermediate scattering function. For the latter the dynamics can not be matched with a single exponential decay, a fact which in the context of experiments is often attributed to the formation of clusters. In this model, it is a consequence of complicated network dynamics.

[1] E. Zaccarelli, F. Sciortino, P. Tartaglia, J. Chem. Phys. 127, 174501 (2007)

CPP 18.9 Mon 18:30 P1C

Cosolvent Effects on Protein Phase Behavior — •Jan Hansen, Florian Platten, and Stefan U. Egelhaaf — Heinrich Heine University, Condensed Matter Physics Laboratory, Duesseldorf, Germany

Cosolvents are routinely used to modulate the stability of proteins. Yet, they also alter protein–protein interactions, which we characterize by static light scattering and in terms of the macroscopic phase behavior of protein solutions. In particular, we experimentally determined the crystallization boundary, the metastable gas–liquid binodal and the second virial coefficient of lysozyme solutions in the presence of various additives, such as sodium chloride (NaCl), guanidine hydrochloride (GuHCl), and glycerol. Our data indicate that the additives might affect the protein phase behavior through electrostatic screening and additive-specific contributions. NaCl induces attractions, glycerol and GuHCl weaken attractions and/or induce repulsions. Using a two-state thermodynamic model, the cosolvent-dependent changes of the phase boundaries can be related to the respective changes of the free energy.

Hansen et al., PCCP, 2016, 18, 10270.

CPP 18.10 Mon 18:30 P1C

Phase behavior of dense lysozyme and nanoparticle solutions — •Julian Schulze[1], Nico König[1], Karin Julius[1], Steffen Bieder[1], Michael Paulus[1], Julia Nase[1], Metin Tolan[1], and Roland Winter[2] — [1]Fakultät Physik/Delta, TU Dortmund, 44221 Dortmund, Germany — [2]Fakultät für Chemie und Chemische Biologie, TU Dortmund, 44221 Dortmund, Germany

In previous studies, small-angle X-ray scattering was used to study the intermolecular interaction potential of lysozyme solutions under the influence of varying environmental conditions such as protein concentration, c, temperature, T, and pressure, p. The attractive part of the interaction potential exhibits a non-monotonous p-dependence with a minimum at ˜ 2 kbar at selected temperatures. Adding NaCl leads to more prominent attractive short range interactions, especially at high c and low T, and the homogeneous protein solution becomes turbid due to the formation of a metastable liquid-liquid phase separated (LLPS) state, where lysozyme forms small droplets of high concentration within a more dilute liquid phase. Due to depletion attraction, Ludox silica nanoparticles show a liquid-liquid phase separation as well when polymers are added. Here, we discuss differences in the mechanism and phase behavior of these dense lysozyme and nanoparticle solutions.

CPP 18.11 Mon 18:30 P1C

Assembly of opal balls on superhydrophobic surfaces — •Lucia Baldauf and Laura Rossi — Universiteit van Amsterdam, Amsterdam, The Netherlands

Colloids are particles with at least one dimension in the size range of 1-1000nm. Since their size is comparable to the wavelengths of visible light, periodic structures of colloidal particles can produce materials with interesting optical properties. When these materials consist of silica spheres organized in highly regular close packed structures, we call them opals. In this work, we investigate the crystallization of silica colloids into opals from evaporating droplets on superhydrophobic surfaces [*Adv. Mat.*, **20**(22), 4263 (2008); *Macromol. Rapid Comm.*, **31**(2), 190 (2010)]. Using superhydrophobic surfaces allows us to induce an isotropic compression of the drying opal balls, rather than introducing a preferential direction by sedimentation under gravity. We study the influence of particle size, shape and surface chemistry on the crystallization process and physical properties of the resulting opals.

CPP 18.12 Mon 18:30 P1C

Self-assembly in solutions of designed supramolecular ferromagnetic filaments — •Ekaterina Novak[1], Pedro Sanchez[2], Elena Pyanzina[1], and Sofia Kantorovich[1,2] — [1]Ural Federal University, Lenin av. 51, Ekaterinburg, 620000, Russia — [2]University of Vienna, Sensengasse 8, 1090, Wien, Austria

Magnetic filaments are semi-flexible polymer-like chains of magnetic nanoparticles permanently crosslinked with polymers which have been recently shown to be promising building blocks for the creation of sophisticated magnetoresponsive materials (Sanchez et al, Faraday Discuss., 2016). Here, we investigate magnetic filaments with different conformations made out of ferromagnetic spherical nanoparticles - simple open chains, closed rings and branched structures with "X" and "Y" junctions - inspired by the recent findings on the low temperature self-assembly and ground state of dipolar hard spheres (Kantorovich et al, PCCP, 2015). Using Langevin dynamics simulations, we focus on low-concentration solutions of filaments, analyzing in detail their self-assembly. Extensive cluster analysis allows to compare the structures formed by filament solutions to those observed in "conventional" magnetic fluids containing non-crosslinked nanoparticles. These results will form the basis for developing theoretical models and provide recommendations for the design of novel magnetoresponsive systems.

CPP 18.13 Mon 18:30 P1C

Investigations of designed supramolecular magnetic filaments of different topology — •Elena Pyanzina[1], Ekaterina Novak[1], Anna Gudkova[1], Pedro A. Sánchez[2], and Sofia Kantorovich[1,2] — [1]Ural Federal University, Lenin av. 51, Ekaterinburg, 620000, Russia — [2]University of Vienna, Sensengasse 8, 1090, Wien, Austria

Newly developed experimental techniques allowed to combine magnetic particles and polymers. These techniques make it possible to create a certain aggregated structures with finely controllable mechanical, magnetic and other properties. Here, we investigate magnetic filaments with different topologies made out of ferromagnetic spherical and ellipsoidal nanoparticles - simple open chains and closed rings which are the ground states of dipolar hard particles (Prokop'eva et al, JETP, 2011; Kantorovich et al, Soft Matter, 2013). Using Langevin dynamics simulations, we analyse different properties of filaments. Thus, we show that shape of particles, the size of their magnetic moment, temperature and filament's length can significantly change conformation and properties of a single filament. These results will form the basis for developing theoretical models and provide recommendations for the design of novel magnetoresponsive systems.

CPP 18.14 Mon 18:30 P1C

Structure and Dynamics of Confined Liquids Studied by an X-ray Surface Force Apparatus — •Henning Weiss[1], Julian Mars[1,2], Hailong Li[1], Hsiu-Wei Cheng[3], Sadhanaa Buvaneswaran[3], Claudia Merola[3], Veijo Honkimaeki[4], Markus Valtiner[3], and Markus Mezger[1,2] — [1]Max-Planck-Institut für Polymerforschung, Mainz, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany — [3]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [4]ESRF-European Synchrotron, Grenoble, France

Confined liquids play an important role in many technical applications and processes. Recent studies on the performance of batteries and capacitors showed that electrochemical and catalytic processes are highly sensitive to the molecular scale liquid structure adjacent to interfaces. Thus, a detailed knowledge of the structure of confined liquids on molecular length scale is of great interest for fundamental and applied sciences. To study confined structures under dynamic conditions we constructed a novel in-situ X-ray surface force apparatus (X-SFA). This device can create a precisely controlled slit pore confinement down to molecular dimensions. The normal load between the apposing interfaces can be modulated to study the structure and dynamics of confined liquids. The in-plane structure of the liquid parallel to the slit pore and density profiles perpendicular to the confining interfaces were studied by X-ray scattering and reflectivity. Relaxation processes were studied by bringing the system out of equilibrium by external stress.

CPP 19: Symposium on Bioinspired Functional Materials: From Nature's Nanoarchitectures to Nanofabricated Designs

Time: Tuesday 9:30–12:15 Location: HSZ 02

Invited Talk CPP 19.1 Tue 9:30 HSZ 02
New twists in biological photonics: circular polarisation and beyond. — •Pete Vukusic, Luke McDonald, and Ewan Finlayson — University of Exeter, Exeter, UK.

The evolution of structural colour mechanisms in many biological systems has given rise to many specialised and often highly functional optical effects both in animals and in plants. Recent scientific works yielded several examples that are being developed for use across technology. Among many thousands of biological systems, a distinctive example involving circular polarisation (CP) was described by Michelson himself: the scarab beetle Chrysina resplendens. Its exoskeleton has a bright, golden appearance that reflects both right-handed and left-handed CP light. The chiral nanostructure responsible for this is a helicoid comprising twisted birefringent dielectric planes. This presentation revisits the C. resplendens beetle, correlating details of its CP reflectance spectra directly with detailed analysis of its morphology that includes a chiral multilayer configuration comprising two chirped, left-handed, helicoids separated by a birefringent retarder. The system's optical behaviour is modelled using a scattering matrix simulation, where the optical roles of each component of the morphological substructure are elucidated. The C. resplendens' model is presented here, alongside summaries of other inspirational biological structural colour generation strategies, as a key example of highly adapted optical design.

Invited Talk CPP 19.2 Tue 10:00 HSZ 02
Bio-inspired materials and structures for technology and architecture — •Thomas Speck — Plant Biomechanics Group & Botanic Garden, University of Freiburg

Biological structures and materials are typically multi-layered, hierarchically structured, finely tuned and highly differentiated based on the combination of a few basic molecular components. This leads to materials and structures that are characterized by multiple networked functions and (often) possess excellent mechanical properties, a pronounced adaptability to changing environmental conditions and manyfold self-x-properties.

During the last decades biomimetics, i.e. using living organisms as inspiration for technical developments products, has attracted increasing attention as well from basic and applied research as from various fields of industry. Biomimetics has a high innovation potential and offers the possibility for the development of sustainable technical products and production chains. On the one hand, novel sophisticated methods for quantitatively analyzing and simulating the form-structure-function-relationship on various hierarchical levels allow new fascination insights in multi-scale mechanics and other functions of biological structures, materials and surfaces. On the other hand, recent developments in computational design and simulation together with new production methods enable for the first time the transfer of many outstanding properties of the biological role models into innovative biomimetic products for reasonable costs which makes them interesting for applications in many fields of technology and building construction.

Invited Talk CPP 19.3 Tue 10:30 HSZ 02
Cellulose bio-inspired hierarchical structures — •Silvia Vignolini — Lensfield Road Cambridge CB2 1EW UK

Nature's most vivid colours rely on the ability to produce complex and hierarchical photonic structures with lattice constants on the order of the wavelength of visible radiation. A recurring strategy design that is found both in the animal and plant kingdoms for producing such effects is the helicoidal multilayers. In such structures, a series of individual nano-fibers (made of natural polymers as cellulose and chitin) are arranged parallel to each other in stacked planes. When distance between such planes is comparable to the wavelength of light, a strong polarised, colour selective response can be obtained. These helicoidal multilayers are generally structured on the micro-scale and macroscopic scale giving rise to complex hierarchical structures.

Biomimetic with cellulose-based architectures enables us to fabricate novel photonic structures using low cost materials in ambient conditions. Importantly, it also allows us to understand the biological processes at work during the growth of these structures in plants. In this talk the route for the fabrication of complex bio-mimetic cellulose-based photonic structures will be presented and the optical properties of artificial structures will be analyzed and compared with the natural ones.

15 min break

Invited Talk CPP 19.4 Tue 11:15 HSZ 02
Strong Flexible Bioenabled Nanocomposites for Sustainable Sensing — •Vladimir Tsukruk — School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, USA

I discuss recent results from our research group on designing flexible and strong responsive polymer and biopolymer nanocomposite materials and structures for advanced flexible sensing and electronic applications. Ultrathin silk fibroin proteins and chemically modified cellulose nanocrystals were assembled in order to control intimate assembly with graphene oxide sheets with controlled surface chemical composition on planar and curved substrates. We demonstrated flexible laminated bionanocomposites with developed biointerphases that facilitate extremely high elastic modulus, bending flexibility, and toughness. Both experimental and computational methods were undertaken to address silk fibroin adsorption at heterogeneous surfaces of graphene oxide with different degrees of oxidation. Graphene oxide and reduced graphene oxide sheets at various levels of oxidation were compared with silicon dioxide (SiO2) as a benchmark substrate. We concluded that silk fibroin readily forms single molecule proto-nanofibrils with β-sheet structures on oxidized graphene oxide surfaces but aggregated globular structures on the hydrophobic surfaces. Finally, electrochemical-assisted photolithography has been utilized for high spatial resolution conductive patterning of these nanocomposites with high local electrical conductivity, sharp boundaries, and optical transparency. Some peculiar features of these flexible bionanocomposites can be explored for tactile recognition, remote sensing, and low-noise SERS substrates.

Invited Talk CPP 19.5 Tue 11:45 HSZ 02
3D laser nano-printing of rationally designed materials — •Martin Wegener — Karlsruhe Institute of Technology, Karlsruhe, Germany

Broadly speaking, 3D structures and materials can be designed by using the human brain, computer-based (topology) optimization, or inspiration from nature. Regardless of how a 3D blueprint has been obtained, it eventually needs to be manufactured. 3D laser printing on the micro- and nanometer scale has become a versatile and reliable workhorse for accomplishing this task. Here, we review recent examples from our group. This includes micropolar metamaterials with behavior beyond ordinary continuum mechanics, metamaterials with effectively negative thermal expansion from positive constituents, and electrical metamaterials with unusual direction and sign of the Hall voltage.

CPP 20: Fundamentals of Perovskite Photovoltaics III (joint session CPP/DS/HL)

Time: Tuesday 9:30–12:30 Location: ZEU 222

Invited Talk CPP 20.1 Tue 9:30 ZEU 222

Investigation of hybrid organic/inorganic perovskite systems and interfaces by photoelectron spectroscopy — •Selina Olthof — University of Cologne, Germany, Luxemburgerstrasse 116, 50939 Cologne

In recent years, the interest in hybrid organic - inorganic perovskites rose at a rapid pace due to their tremendous success in the field of photovoltaics. In addition to the thin film properties of the active layer, the performance of optoelectronic devices strongly depends on the appropriate energetic alignment between the active- and adjacent layers. In order to choose adequate transport materials for the increasingly complex hybrid perovskite compositions in a non-trial-and-error fashion, it is important to understand how the induced changes in band gap relate to shifts in the valence and/or conduction band.

In this talk, I will discuss recent findings regarding measurements of the electronic structure of various hybrid perovskites, covering lead as well as tin based systems and a variety of halogens using UV-, inverse, and x-ray photoelectron spectroscopy measurements (UPS/IPES/XPS). Furthermore, using these surface sensitive techniques the alignment at interfaces between different layers can be probed in-situ as well by performing a stepwise film preparation. Looking at various bottom contacts we find that chemical interactions, band bending, and interface dipole formation play an important role. Therefore, the nature of the substrate not only determines the energetic alignment but can lead to chemical reactions and influence film formation and crystallinity.

CPP 20.2 Tue 10:00 ZEU 222

Influence of air and water on the electronic structure of CH3NH3PbI3-xClx mixed halide perovskite film surfaces — •Maryline Ralaiarisoa, Fengshuo Zu, and Norbert Koch — Humboldt-Universität zu Berlin, Institut für Physik & IRIS Adlershof, Brook-Taylor-Str. 6, 12489 Berlin, Deutschland

Water and oxygen under environmental conditions reveal to be both beneficial for device performance as well as detrimental to the stability of perovskite based solar cells and films. Within this controversy, an accurate and comprehensive description of the influence of these factors is still lacking, particularly on the electronic structure of perovskite films. We investigated the effect of water and air on the ionization energy (IE) and the electronic structure of perovskite films. To this end, we used photoelectron spectroscopy to monitor the electronic structure of perovskite films following a range of procedures, including thermal post-treatment, as well as air and oxygen exposure. After air exposure, we observe changes of work function (WF) and IE similar to those after pure oxygen exposure. Furthermore, our observations indicate that even without prior ambient air exposure residual water (from processing in a typical glove-box environment) can still be present on the surface of perovskite films, even under vacuum conditions. Such water adsorption seemingly increases the WF of the perovskite films. Our results underline how environmental conditions substantially affect the electronic structure of perovskite films, which will likely impact the energy level alignment in perovskite-based photovoltaic cells.

CPP 20.3 Tue 10:15 ZEU 222

Modulated surface photovoltage spectroscopy of CH3NH3Pb(I,Br)3 thin films — •Celline Awino, Thomas Dittrich, Eva Unger, and Bernd Rech — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium-Photovoltaik, Kekuléstr. 5, 12489 Berlin, Deutschland

The investigation of electronic properties of CH3NH3Pb(I,Br)3 and their dependence on aging and light soaking is important for better understanding of the stability of solar cells based on related materials. Modulated surface photovoltage spectroscopy allows for the ex-situ and in-situ characterization of the band gap, tail states and deep defect states in the band gap, direction of modulated charge separation and diffusion length. It has been found, for example, that the Tauc gap and the energy of exponential tail states sensitively depend on the substrate and on soaking in nitrogen atmosphere and that light soaking has strong influence on the direction and amplitude of modulated charge separation.

CPP 20.4 Tue 10:30 ZEU 222

Revealing the impact of the potential distribution within high performing Lead Methylammonium Tri-Iodide solar cells with organic contact materials — •Christian Müller[1,2,3], Bernd Epding[2,3], Ramos Bwalya[2,3], Michele Sessolo[4], Lidón Gil-Escrig[4], Henk Bolink[4], Robert Lovrincic[1,3], and Wolfgang Kowalsky[1,2,3] — [1]IHF, TU Braunschweig, Germany — [2]KIP, Universität Heidelberg, Germany — [3]InnovationLab, Heidelberg, Germany — [4]Instituto de Ciencia Molecular, Universidad de Valencia, Spain

Over the last few years the power conversion efficiency of organometal-halide perovskite (such as $CH_3NH_3PbI_3$, MAPI) based solar cells has skyrocketed at an unprecedented rate to values around 22%. However, the understanding of the physical process in the solar cells drags behind the progress of efficiency. For example, the influence of the potential distribution in such cells on their performance is so far not sufficiently studied.

We focus in this work on high performing fully vacuum processed MAPI solar cells with organic contact materials [1]. We will present SKPM measurements on p-i-n and n-i-p solar cell cross sections that map the potential distribution within the device with high spatial resolution. Performing measurements under different conditions enables us to determine the influence of potential barriers at the contact interfaces and of a poling on the cell efficiency.

[1] Energy Environ. Sci., 2016, 9, p. 3456-3463, C. Momblona et al.

CPP 20.5 Tue 10:45 ZEU 222

Impact of Illumination on the Electronic and Chemical Structure of Mixed Halide Perovskites — •Fengshuo Zu[1], Patrick Amsalem[1], Ingo Salzmann[1], Rongbin Wang[1,2], Maryline Ralaiarisoa[1], Stefan Kowarik[1], Steffen Duhm[2], and Norbert Koch[1] — [1]Institut für Physik,Humboldt-Universität zu Berlin,12489 Berlin,Germany — [2]FUNSOM,Soochow-University,Suzhou,China

The seemingly n-type behavior of the perovskite films is largely intriguing since these films are calculated to be bipolar conductive. For exploring the fundamental physics of the n-type behavior, we investigate the effect of white-light illumination on the electronic structure of mixed halide perovskite thin films and of CH3NH3PbI3 single crystals using X-ray and ultraviolet PES, as well as UV-Vis absorption spectroscopy. The samples are found to be strongly n-type and, upon illumination, the valence band features shift by up to 0.7 eV to lower BE. We show this effect to be correlated with initial surface band bending due to the presence of donor levels likely consisting of reduced lead (Pb0) acting as surface traps. Upon short-time illumination, this phenomenon is found to be partially reversible, for prolonged illumination, however, a high concentration of metallic Pb0 is generated inducing strong Fermi-level pinning. This effect is accompanied by the formation of PbI2 defects within the film and a deficiency of iodine in the surface region. Experiments performed on CH3NH3PbI3 single crystal reveal the presence of a relatively high concentration of reduced Pb0 at the sample surface after cleaving, likewise, strongly pinning the Fermi-level even under high intensity illumination.

15 min break

CPP 20.6 Tue 11:15 ZEU 222

Giant Rashba Splitting in $(CH_3NH_3)PbBr_3$ Organic-Inorganic Perovskite — Daniel Niesner[1], Max Wilhelm[1], Ievgen Levchuk[2], Andres Osvet[2], Shreetu Shrestha[2], Miroslaw Batentschuk[2], Christoph Brabec[2,3], and •Thomas Fauster[1] — [1]Lehrstuhl für Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [2]I-MEET, Department of Materials Science and Engineering, FAU Erlangen-Nürnberg, Martensstr. 7, D-91058 Erlangen, Germany — [3]ZAE Bayern, Haberstr. 2a, D-91058 Erlangen, Germany

A Rashba-type spin-split band structure has been predicted for organic-inorganic perovskite semiconductors. The effect has been proposed as one of the origins of the exceptionally long carrier lifetimes in the materials, forming the basis of their successful application in optoelectronics. Using angle-resolved photoelectron spectroscopy, we investigate the band structure of $(CH_3NH_3)PbBr_3$ single crystals cleaved in ultrahigh vacuum. The orthorhombic low-temperature phase and the cubic room-temperature phase are studied. We apply a modified leading-edge method to identify the dispersion of the valence band edge. It reveals two valence band maxima, separated in k-space by 0.043 $Å^{-1}$. The dispersion is indicative of Rashba splitting. This interpretation is supported by the observation of circular dichroism in the orthorhombic phase. Extracted Rashba parameters of $\alpha_o = 7 \pm 1$ eV Å and $\alpha_c = 11 \pm 4$ eV Å in the orthorhombic and the cubic phase are amongst the largest reported to date.

CPP 20.7 Tue 11:30 ZEU 222

Exploring the electronic band structure of (organo-)metal halide perovskite via photoluminescence anisotropy of individual nanocrystals — •Daniela Täuber[1], Mirko Goldmann[1,2], Juanzi Shi[1], Alexander Dobrovolsky[1], and Ivan Scheblykin[1] — [1]Chemical Physics, Lund University, Lund, Sweden — [2]TU Ilmenau, Germany

Understanding electronic processes in metal halide perovskites requires unraveling the origin of their electronic transitions. Light polarization studies can provide important information regarding transition dipole moment orientations. Investigating individual lead trihalide perovskite nanocrystals enabled us to detect the polarization of photoluminescence intensity and photoluminescence excitation, hidden in bulk samples by ensemble averaging. Polarization properties of $CH_3NH_3PbI_3$ crystals were correlated with their photoluminescence spectra and electron microscopy images [1]. We propose that distortion of PbI6 octahedra leads to peculiarities of the electronic band structure close to the band-edge. Namely, the lowest band transition possesses a transition dipole moment along the apical Pb-I-Pb bond resulting in polarized photoluminescence. Excitation of photoluminescence above the bandgap is unpolarized because it involves molecular orbitals delocalized both in the apical and equatorial directions of the perovskite octahedron. Trap-assisted emission at 77 K, rather surprisingly, was polarized similar to the bandgap emission.

D.T. acknowledges a personal research grant DFG-TA 1049/1-1.

[1] Täuber, D. et al., Nano Letters 16, 5087-5094, 2016.

CPP 20.8 Tue 11:45 ZEU 222

Band Edge Engineering of Hybrid Halide Perovskites for Solar Cell Applications - Insights from Density Functional Theory — •Linn Leppert[1,2], Sebastian E. Reyes-Lillo[1,2], and Jeffrey B. Neaton[1,2,3] — [1]Molecular Foundry, Lawrence Berkeley National Laboratory — [2]Department of Physics, University of California Berkeley — [3]Kavli Energy NanoScience Institute at Berkeley

Efficiencies of solar cells based on hybrid halide perovskite absorbers have reached 22%, making them serious contenders to silicon solar cells. Nevertheless, the toxicity of lead, the material's instability, as well as pressing questions about the role of structural heterogeneities present challenges to its large scale fabrication and long term use. Recently it has been shown that photovoltaic properties vary significantly between different crystal facets of perovskite thin films, suggesting an appreciable effect of electric fields on the local electronic structure [1]. In this contribution, I will elucidate the coupling between electric polarization, which increases as a function of the macroscopic alignment of the organic moieties, and the band edge electronic structure. In particular the Rashba effect, an energy band splitting in k-space, increases with increasing polarization, indicating significant tunability with experimentally feasible applied fields. The effect can be tuned further by chemical substitution of the organic molecule as well as by anisotropic strain, allowing for considerable Rashba splitting even in the absence of electric fields [2]. [1] S. Leblebinci, L. Leppert, et al., Nature Energy 1, 16093 (2016). [2] L. Leppert et al., J. Phys. Chem. Lett. 7, 3683 (2016).

CPP 20.9 Tue 12:00 ZEU 222

Computational serach for sulphide perovskites for solar energy conversion application — •Korina Kuhar, Mohnish Pandey, Kristian Sommer Thygesen, and Karsten Wedel Jacobsen — Center for Aromic-scale Materials Design (CAMD), Department of Physics, Technical University of Denmark, DK * 2800 Kgs. Lyngby, Denmark

Oxide perovskites are in general known to be wide band gap semiconductors which hampers their use for visible light absorption. However, recent experiments on the synthesis of inorganic sulphide perovskites, for example BaZrS3[1] and SrZrS3[2], with band gaps of 1.7 ev and 0.8-1 eV, respectively, show that sulphur is a possible supstitution to oxygen in inorganic perovskites to lower their band gaps. Several binary, ternary and quaternary sulphides are already known to have relevant band gaps. We perform a systematic investigation of the class of ABS3 compounds in eight phases using Density Functional Theory (DFT). The screening procedure applied is based on simple criteria such as stability, band gap in the visible part of the solar spectrum, high charge mobility and small tendency of the material to form defects. Finally we report a set of sulphide perovskites we found to be stable and have interesting properties for use as solar energy conversion materials.

1. DOI: 10.1021/acs.chemmater.5b04213 2. DOI: 10.1016/j.solidstatesciences.2005.02.010

CPP 20.10 Tue 12:15 ZEU 222

Towards a multiscale statistical description of hybrid perovskite materials — •Jingrui Li[1], Jari Järvi[1,2], and Patrick Rinke[1] — [1]COMP Centre of Excellence, Aalto University, Finland — [2]Department of Physics, University of Helsinki, Finland

Hybrid perovskites (HPs), in particular methylammonium lead iodide ($MAPbI_3$), have received enormous interest in recent years as promising photoactive materials in emergent photovoltaic technologies. An important feature of HPs is their structural complexity introduced by the organic cations (e.g., MA^+). At room temperature or above, the MAs will be oriented (quasi-)randomly, forcing HPs into disordered structures. The disorder affects important materials properties such as the stability and electronic structure that are crucial for the application of HPs in novel photovoltaic devices. Our previous density-functional theory (DFT) study reveals that hydrogen bonding leads to an anisotropic interaction between the MA cations and the inorganic cage. The deformed cage and the MA orientation are interdependent, analogous to a chicken-and-egg paradox [1]. From the insight of this single unit cell model, we derive a multiscale scheme for disordered $MAPbI_3$ structures, in which the interaction between neighbouring MA ions is described by a pair model. We show that the total number of relevant pairs can be reduced to only 86 and then analyse DFT results for large, geometry optimized $MAPbI_3$ supercell models in terms of their "pair-mode" distribution. With our model we can then describe disordered HPs on length scales beyond a few nanometers.

[1] J. Li and P. Rinke, *Phys. Rev. B* **94** 045201 (2016).

CPP 21: Organic Electronics and Photovoltaics III: Mobile and Trapped Charges (joint session CPP/DS/HL, organized by CPP)

Time: Tuesday 9:30–12:45 Location: ZEU 260

CPP 21.1 Tue 9:30 ZEU 260

A Kelvin-Probe study of the electrical transport in organic semiconductors — •Karl-Philipp Strunk[1], Valeria Milotti[1], Alexander Ullrich[2], and Christian Melzer[1] — [1]Centre for Advanced Materials, University of Heidelberg, Germany — [2]Chemiches Institut, Universität of Heidelberg, Germany

DC current-voltage measurements on organic field-effect transistors (organic FET or OFET) are commonly used to characterize the planar electrical transport in organic semiconductors. In this study we report an alternative AC dark-injection method giving likewise access to in-plane transport parameters of organic semiconductor thin films. Exposing a macroscopic FET-like structure to a periodic bias leads to a periodic change in surface potential which can be tracked via a Kelvin-Probe giving direct insight into the movement of lateral charge-carrier waves along the organic film. Tracking the temporal evolution of the surface potential distribution allows for the determination of the charge-carrier mobility at low currents, a regime which is conventionally hardly accessible. It will be shown that this regime allows for a mobility determination at P3HT based devices fairly independent on contact properties. In order to elucidate the influences of electrical properties like doping concentration, traps states and injection barriers on the device response, time-dependent finite-element simulations have been carried out.

CPP 21.2 Tue 9:45 ZEU 260

Spin dynamics and spin current in a high-mobility polymer — •Thorsten Arnold[1], Andreas Lücke[2], Uwe Gerstmann[2], Wolf Gero Schmidt[2], and Frank Ortmann[1] — [1]Institute for Materials Science, Center for Advancing Electronics Dresden and Dresden Center for Computational Materials Science, Technische Universität Dresden, 01069 Dresden, Germany — [2]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany

Organic semiconductors are characterized by small spin-orbit coupling, which leads to a relatively long spin relaxation time. This makes them particularly interesting materials for spintronics. We describe spin transport in the thiophene-based polymer PBTTT using a recently developed generalization of the Kubo formalism to spin and an appropriate definition of the spin current operator in tight-binding form to investigate the spin conductivity tensor in PBTTT. The transfer integrals of the Hamiltonian and spin current operator are extracted from the DFT band structure with and without spin-orbit coupling. The spin propagation and spin conductivity for different spin-orbit transfer integral models are compared and the energy dependence and relaxation are analyzed.

CPP 21.3 Tue 10:00 ZEU 260

Virtual screening for high carrier mobility in organic semiconductors — •Christoph Schober, Karsten Reuter, and Harald Oberhofer — Technische Universität München

Low carrier mobilities still hamper the use of organic semiconductors in many applications. Using a staged virtual screening approach we compute the electronic couplings and intramolecular reorganization energies as two main descriptors for charge mobility for a set of 95445 molecular crystals extracted from the Cambridge Structural Database (CSD). Descriptor calculations are performed using efficient density functional theory methods developed in our group, together with a fully automated workflow system for data preparation and verification. As a final step, based on the calculated coupling values we identify materials with long-range charge percolation pathways. We readily find many acclaimed compounds, as well as a number of most promising materials that have not yet been considered for an application in organic electronics. Together with the unique meta-data provided in the CSD the large descriptor database allows to extract important trends and correlations that will further accelerate the theoretical design and discovery of high mobility organic semiconductors.

C. Schober, K. Reuter, H. Oberhofer, *J. Chem. Phys.* **2016**, *144*, 054103.

C. Schober, K. Reuter, H. Oberhofer, *J. Phys. Chem. Lett.* **2016**, *7*, 3973-3977.

CPP 21.4 Tue 10:15 ZEU 260

Utilizing Schottky barriers to suppress short channel effects in organic transistors — •Antón F. Fernández and Karin Zojer — Institute of Solid State Physics and NAWI Graz, Graz University of Technology, Graz, Austria

High switching speeds constitute one of the optimization targets for organic thin film transistors (OTFT). Reducing the channel length is a major handle to boost the switching speed of OTFTs. However, upon reducing the channel length one has to cope with undesired short-channel effects, i.e., a loss of saturation, a reduced ON-OFF ratio, and a disproportionally larger impact of the contact resistance. We demonstrate by virtue of device simulations that the ON-OFF-ratio of a short channel transistor is enhanced by orders of magnitude when a Schottky barrier at the injecting contact is intentionally introduced. The key effect is the efficient suppression of the OFF-current while trading in only a small loss in the ON current. We show that, in fact, it is possible to establish a minimal Schottky barrier such that the short channel transistors can be operated without premature turn-on while retaining an ON current as large as expected from Gradual Channel approximation. This strategy is suited for staggered and coplanar transistor architectures.

CPP 21.5 Tue 10:30 ZEU 260

Direct Au-C contacts based on biphenylene for single molecule transport — •Narendra P. Arasu and Héctor Vázquez — Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10/112, Prague, Czech Republic

Metal-molecule contacts strongly influence the mechanical, electronic and conducting properties of molecular junctions [1]. Here we use Density-Functional Theory (DFT) and Non-Equilibrium Green's Function (NEGF) methods to study biphenylene-based molecular circuits. We expect that at the Au surface the biphenylene molecule will break a weak intramolecular C-C bond and form covalent bonds to the substrate. Direct Au-C metal-molecule links were shown to be highly-conducting [2,3]. With these Au-C links to the substrate, we then consider several linker groups at the other end of the molecule, which is contacted by a Au tip. We calculate the mechanical properties of the junctions from tip approach trajectories and find that Au-C bonds are stable under the stress induced by the approaching tip. We then discuss the conductance of the junction focusing on the dependence of transport behaviour on linker chemistry.

[1] F. Schwarz et al., J. Phys.: Condens. Matter 26, 474201 (2014).
[2] Z. L. Cheng et al., Nat. Nanotechnol 6, 353-357 (2011).
[3] W. Chen et al., J. Am. Chem. Soc 133, 17160 (2011).

CPP 21.6 Tue 10:45 ZEU 260

Controlling the transport in organic electronics via self-assembled Monolayers — •Anja Förster[1], Sibylle Gemming[2,3], and Gotthard Seifert[1] — [1]TU Dresden, Center for Advancing Electronics Dresden (cfaed), 01062 Dresden, Germany — [2]Institute of Ion Beam Physics and Material Research, Helmholtz-Zentrum Dresden Rossendorf, Center for Advancing Electronics Dresden (cfaed), Bautzner Landstr. 400, 01328 Dresden, Germany — [3]Insitute of Physics, TU Chemnitz, 09107 Chemnitz, Germany

Self-assembled monolayers (SAM) can be used to control the transport in organic field-effect transistors. The SAM creates a dipole moment induced electric field that is able to change the major transport type in organic materials.

In the case of fluoroalkyl SAMs, their strong dipole moment induces electric fields up to 10^9 V/m. These fields are strong enough to affect the underlying organic material up to a distance of 10-20 Å from the SAM. Due to the orientation of the dipole moments this leads to a hole dominated transport.

Amine-based SAMs, on the other hand, enhance the electron transport as their dipole moment is counter-directional to the one from fluoroalkyl SAMs. Due to their lower absolute dipole moment, their effect is not as strong as for fluoroalkyl SAMs.

Finally, we exemplarily show for pentacene how the SAM molecules connect to the organic material. The resulting distance of the SAM layer to the organic material determines the maximum strength of the dipole moment induced electric field.

15 min break

CPP 21.7 Tue 11:15 ZEU 260

Electronic components embedded in a single graphene nanoribbon — •Peter Jacobse[1,2], Fabian Schulz[3], Adri van den Hoogenband[2], Marc-Etienne Moret[2], Robertus Klein-Gebbink[2], Peter Liljeroth[3], and Ingmar Swart[1] — [1]Debye Institute for Nanomaterials Science, Utrecht University, PO Box 80000, 3508 TA Utrecht, The Netherlands — [2]Princetonplein 1 — [3]2Department of Applied Physics, Aalto University School of Science, PO Box 15100, 00076 Aalto, Finland

On-surface synthesis offers a convenient route to atomically well-defined graphene nanoribbons (GNRs) with a precisely controlled width and edge structure. In addition to monocomponent ribbons, GNR heterojunctions joining two semiconducting segments with different band gaps (through ribbon width) or different band-alignment (through nitrogen substitution) have been demonstrated. The driving force in this direction is to build more functionality into a single ribbon for applications in GNR-based electronics or photovoltaics. However, the GNR equivalents of a metal-semiconductor junction or a tunnel barrier have not yet been realized. We embed these junctions in a single GNR by joining armchair GNRs belonging to the metallic (5-atom wide) and semiconducting (7-atom wide) families through on-surface synthesis. We characterize the atomic scale geometry and electronic structure by combined atomic force microscopy (AFM), scanning tunneling microscopy (STM) and conductance measurements. The GNR equivalent of a tunnel barrier constitutes a first step towards complete electronic devices built into a single GNR.

CPP 21.8 Tue 11:30 ZEU 260

Thermoelectric thin films based on a polymer/nanoparticle nanocomposite — •Nitin Saxena[1,2], Mihael Coric[3], Anton Greppmair[4], Jan Wernecke[5], Mika Pflüger[5], Michael Krumrey[5], Martin S. Brandt[4], Eva M. Herzig[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, Munich School of Engineering, 85748 Garching, Germany — [4]TU München, Walter-Schottky-Institut and Physik-Department, 85748 Garching, Germany — [5]PTB, BESSY II Helmholtz-Zentrum Berlin, 12489 Berlin, Germany

Thermoelectric materials pose a compelling technology for power generation from renewable energies, since temperature gradients are transformed into voltages and thus electrical power. So far, highly efficient thermoelectrics comprise rare and/or toxic inorganic materials, and require cost- and energy-intensive fabrication. These points hinder their large-scale application. 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. Beside the thermoelectric properties, we investigate the thermal conductivity of pristine PEDOT:PSS and of the hybrid film, in order to ultimately calculate the figure-of-merit ZT. Tender resonant x-ray scattering (T-ReXS) is used to derive a morphological model, and describe the influence of the nanoparticles on the thermoelectric properties.

CPP 21.9 Tue 11:45 ZEU 260

Modelling long-term isothermal charge decay in modified PTFE electrets — •Dmitry Rychkov — University of Potsdam, Potsdam, Germany

Electret stability is usually best characterised by means of charge decay as a function of time. In highly stable electret materials, charge-decay measurements require very lengthy experiments even at elevated temperatures. Isothermal charge-decay curves, however, can be modelled if thermally-stimulated discharge data are known. Here, we attempt to deal with this problem for electrets made from chemically modified polytetrafluoroethylene (PTFE) films. PTFE films were treated with TiCl4 vapor in a flow-type reactor and electrically charged in a positive corona discharge. Using the charge-transport theory by Simmons, frequency factors and energy spectra for the relevant surface traps have been extracted from thermally stimulated surface-potential decay curves. The data were then used to calculate isothermal charge-decay curves at different temperatures. A detailed comparison between the modelled and the experimental curves reveals good agreement at elevated temperatures. At lower temperatures, however, the modelled isothermal charge-decay curves deviate from the experimental ones and show a slower decay, which indicates that additional mechanisms that are not covered in the theory may contribute to the electret-charge decay in this temperature range. We propose a simple phenomenological model to illustrate the effects of such mechanisms and to determine the applicability limits of our charge-decay modelling method.

CPP 21.10 Tue 12:00 ZEU 260

Large area three-dimensional polarization control in P(VDF-TrFE) polymer films on graphite — •Robert Roth[1], Martin Koch[1], Jakob Schaab[2], Martin Lilienblum[2], Thomas Thurn-Albrecht[1], and Kathrin Dörr[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, 06099 Halle, Germany — [2]Department of Materials, ETH Zürich, Vladimir-Prelog-Weg 1-5/10, 8093 Zürich, Switzerland

Ferroelectric polymers are attractive candidates for functional layers in electronic devices like non-volatile memories, piezo- and magnetoelectric sensors, and capacitor-based high speed energy storage devices. Unfortunately, such thin films often reveal low di- and piezoelectric responses due to reduced crystalline and electrical dipole order, leading to compensation effects and low effective electric performance. One of the best characterized and often applied ferroelectric polymers is poly(vinylidene fluoride-co-trifluoroethylene) (P(VDF-TrFE)). We will present results on micron-sized domains with three dimensional ferroelectric polarization alignment in P(VDF-TrFE) films on graphite. The ferroelectric domains have been achieved by a combined procedure of electrical poling and mechanical annealing with an atomic force microscopy tip. They show strongly increased lateral and vertical piezoresponse compared to the as-prepared film and can be deliberately written and switched.

CPP 21.11 Tue 12:15 ZEU 260

Significanlty enhanced charging efficiency for higher piezoelectricity in polymer ferroelectrets — •Xunlin Qiu — Department of Physics and Astronomy, University of Potsdam, 14469 Potsdam, Germany

Ferroelectrets are internally charged polymer foams or cavity-containing polymer-film systems. They are charged through a series of dielectric barrier discharges (DBDs) inside the cavities which interact with the internal polymer surfaces [1]. The breakdown strength of the gas strongly influences the charging process. A gas with a lower breakdown strength has a lower charging voltage, but leads to a lower remanent polarization. Charging in gases with higher breakdown strength requires higher voltage but allows higher remanent polarization. Here, a charging scheme involving gas exchange during charging is proposed [2]. The cavities of a tubular-channel fluoroethylenepropylene (FEP) ferroelectret are first filled with helium (lower breakdown strength), so that DBDs can be easily triggered by applying a relatively low voltage. The charging voltage should not be turned off until the gas inside the cavities has been replaced with nitrogen or air (having higher breakdown strength), in order to achieve higher remanent polarization. With the proposed charging scheme, the charging efficiency and hence the resultant piezoelectricity of ferroelectrets can be significantly enhanced.

[1] X. Qiu, W. Wirges and R. Gerhard, J. Appl. Phys. 110, 024108 (2008).

[2] X. Qiu, Appl. Phys. Lett. 109, 222903 (2016).

CPP 21.12 Tue 12:30 ZEU 260

Tuning the Electronic Properties of 3D Covalent Organic Networks by Collective Electrostatic Design — •Veronika Obersteiner, Andreas Jeindl, Johannes Götz, Aurelie Perveaux, and Egbert Zojer — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

Covalent organic frameworks have recently attracted substantial interest as materials for photovoltaics applications, as they can be synthesized mimicking donor-acceptor bulk heterojunctions.

On the basis of first-principle results we propose a novel design strategy for analogous 3D organic networks, where a band offset between different semiconducting segments can be achieved by introducing periodic arrangements of dipolar elements into the material. Exploiting the resulting collective electrostatic effects, we are able to manipulate the electronic landscape of the 3D networks in a controlled way,thereby, achieving spatially confined pathways for electrons and holes. The distinct advantage of this approach over conventional strategies for achieving the band offset by using chemically distinct donor and acceptor units is that the magnitude of the band offset can be tuned continuously. The suggested electrostatic design strategy also enables the realization of more complex structures like quantum-cascades and 'quantum-checkerboards'.

CPP 22: Polymer Networks and Dynamics II: Structure and Dynamics

Time: Tuesday 9:30–12:45 Location: ZEU 250

CPP 22.1 Tue 9:30 ZEU 250

Local orientational mobility in regular fractal networks — •Maxim Dolgushev[1,2], Denis A. Markelov[3,4], Florian Fürstenberg[1], and Thomas Guérin[5] — [1]Institute of Physics, Uni Freiburg, Germany — [2]Institut Charles Sadron, Strasbourg, France — [3]St. Petersburg State University, Russia — [4]ITMO University, St. Petersburg, Russia — [5]LOMA, CNRS UMR 5798, Talence, France

This contribution presents the study of the local orientational dynamics of single bonds in fractal networks with the focus on the location of the bonds [1]. In contrast to studies on overall or structurally averaged dynamics, which typically need only the eigenvalues of the dynamical matrix, the investigation of the local dynamics requires the calculation of the coefficients from the eigenvectors of this matrix. To overcome this difficulty we provide iterative methods for calculation of such coefficients. The suggested procedure allowed us to treat very large structures (which would not be accessible by naive brute force diagonalization procedures) and to investigate the corresponding scalings for the dielectric relaxation. We show that the local dynamics can be vastly different from the structure averaged one. Indeed, the dynamics of the core segments (which are most remote from the periphery) has a scaling behavior, which differs from the dynamics obtained after structural average. Moreover, we analyze the most relevant processes of single segment motion and provide a well performing analytic approximation for the corresponding relaxation times.

[1] M. Dolgushev, D. A. Markelov, F. Fürstenberg, T. Guérin, Phys. Rev. E. 94, 012502 (2016).

CPP 22.2 Tue 9:45 ZEU 250

Dynamics of internally functionalized dendrimers — •Jonas Grimm[1] and Maxim Dolgushev[1,2] — [1]Institute of Physics, Uni Freiburg, Germany — [2]Institut Charles Sadron, Strasbourg, France

Recently, new types of dendrimers have been synthesized; among them the internally functionalized dendrimers are of a particular interest. We analyze the dynamics of such functionalized dendrimers that have additional functional units, which do not branch out further.

The dendrimers are modeled in the framework of semiflexible tree-like polymers [1], where their topology is described through beads connected by springs (bonds) and semiflexibility is taken into account by constraining the bonds' orientations. The dynamics of the structures is described by a set of Langevin equations. The spectrum of the dynamical matrix appearing in these equations is fundamental for the dynamical properties. In particular, the additional functional beads clearly leave their fingerprints in the eigenvalue spectrum of the dynamical matrix: We find a group of eigenvalues which does not exist for homogeneous dendrimers [2]. This part of the spectrum leads to an additional process in the intermediate frequency region of the imaginary part of the complex dielectric susceptibility. The presence of functional beads is clearly manifested in the local dynamics of the non-functionalized segments on intermediate frequencies [2].

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

[2] J. Grimm and M. Dolgushev, Phys. Chem. Chem. Phys.18, 19050 (2016).

CPP 22.3 Tue 10:00 ZEU 250

Glassy dynamics in one- and two-dimensional nanometric confinement - a comparison — •Friedrich Kremer and Wycliffe K. Kipnusu — Institute of Experimental Physics I, University of Leipzig, 04103 Leipzig, Germany

Glassy dynamics of polymers (e.g. poly(methylphenylsiloxane) (PMPS) or poly(cis1,4-isoprene) (PI)) is studied by broadband dielectric spectroscopy (BDS) in one-(1D)- and two-(2D)-dimensional nanometric confinement; the former is realized in thin layers having thicknesses down to 5 nm, the latter in unidirectional (length 50 m) nanopores with diameters varying between 4-8 nm. Based on dielectric measurements carried out in a broad spectral range at widely varying temperatures glassy dynamics is analyzed in detail in 1D and in 2D confinement. All the findings can be comprehended by considering the density of the polymer; in 1D it is assumed to be the same as in the bulk, hence the dynamic glass transition is not altered, in 2D it is reduced due to a frustration of packaging resulting in a higher free volume, as proven by ortho-positronium annihilation lifetime spectroscopy. [1] "Dynamics in Geometrical Confinement", F. Kremer (Ed.), Springer (2014) [2] Kipnusu, W.K. et al., "Glassy dynamics of polymethylphenylsiloxane in one-and two-dimensional nanometric confinement-a comparison", submitted 2016 [3] Kipnusu, W.K., "Confinement for More Space: A Larger Free Volume and Enhanced Glassy Dynamics of 2-Ethyl-1-hexanol in Nanopores" J. Phys. Chem. Lett. 6, 3708-3712 (2015) [4] Kipnusu, W.K., et al. "Structure and Dynamics of Asymmetric Poly(styrene-b-1,4-isoprene) Diblock Copolymer under 1D and 2D Nanoconfinement" ACS Appl. Mater. Interfaces, 7, 12328-12338 (2015) [5] Mapesa, E.U., et al. "Molecular dynamics of poly(cis-1,4-isoprene) in 1- and 2-dimensional confinement" in: "Dynamics in Geometrical Confinement", F. Kremer (Ed.), Springer (2014)

CPP 22.4 Tue 10:15 ZEU 250

Tuning polymer dynamics by chain-end association — •Martin Tress[1], Kunyue Xing[1], Pengfei Cao[2], Shiwang Cheng[2], Tomonori Saito[2], Vladimir Novikov[1], and Alexei Sokolov[1,2] — [1]University of Tennessee Knoxville — [2]Oak Ridge National Laboratory

Functional end groups in polymers are a molecular tool to reversibly connect and disconnect chains to combine properties of both short polymer and large supramolecular structures. The topology of the latter - and in turn the respective properties - can be tuned by the choice of the functional group. This is shown in a series of polydimethyl siloxanes (PDMS) of different molecular weight (MW) which are terminated by amino and carboxylic (-COOH) groups, respectively. Differential scanning calorimetry and dielectric spectroscopy measurements reveal that segmental dynamics are identical for the chains with two different end groups. In contrast, rheology unravels a mechanical reinforcement for PDMS-COOH and a rise in viscosity by ~2 decades. This is accompanied by a 2nd Tg and a corresponding dielectric relaxation process which indicates phase separation of the end groups in clusters forming a physically crosslinked network. As a consequence, the viscoelastic properties can be tuned from common short polymer chains at high temperatures to highly entangled or even crosslinked systems at T close and below the 2nd Tg. This suggests a promising route to combine easy processibility of low MW polymers with the desired mechanical performance of high MW polymers or even crosslinked networks.

CPP 22.5 Tue 10:30 ZEU 250

Cross-link fluctuations in entangled networks — •Michael Lang — Leibniz-Institut für Polymerforschung, Hohe Straße 6, 01069 Dresden, Germany

Cross-link fluctuations affect the instantaneous and time average bond orientations in entangled networks that are measured as birefringence or by Nuclear Magnetic Resonance respectively. In order to develop a quantitative model for cross-link fluctuations, computer simulation data on junction fluctuations in end-linked model networks are analyzed using the framework of the constrained junction model and the slip tube model of entangled networks. We discuss an analytical expression for cross-link fluctuations that compares well with simulation data on elasticity and residual bond orientations. As a consequence, cross-link fluctuation data can be used to estimate the tube diameter.

CPP 22.6 Tue 10:45 ZEU 250

A novel route towards entropic polymer separation — •Paolo Malgaretti — Max Planck Institute for Intelligent Systems, Heisenbergstr. 3 70569 Stuttgart Germany

Many biological processes such as viral infection, DNA transport through membranes and gene transferring between bacteria involve the translocation of bio-polymer through nano-channels and nano-pores. Moreover, technological applications such as polymer separation, DNA sequencing, and protein sensing, rely on the translocation of polymer through restrictions.

Up to now, much attention has been payed to the case of polymers translocating through pores whose half-section is comparable to the monomer size. In contrast to this, we are concerned with the case of a polymer translocating through channels, whose cross section is larger than the size of a single monomer, yet comparable to the size of the overall gyration radius of the polymer.

In such a regime a novel dynamical scenario occurs and it appears a non-monotonous dependence of polymer translocation velocity as a function of polymer size, a feature that can be exploited for polymer separation. I will show that these numerical results can be rationalized on the basis of a simplified model that reduces the problem of polymer translocation through varying-section channels to that of a point-like particle under the action of an effective potential.

15 min break

Invited Talk CPP 22.7 Tue 11:15 ZEU 250

Structure/dynamics interplay in interfacial layers: how adsorption influences thermal glass transition and segmental relaxation — •Simone Napolitano — Université Libre de Bruxelles (ULB), Brussels, Belgium

Growing experimental evidence shows that the behavior of thin polymer layers strongly depends on the degree of adsorption, the number density of monomers pinned onto the supporting substrate. Several groups have independently observed that properties as wettability, viscosity and thermal expansion are affected by prolonged annealing in the liquid state, even at timescales exceeding the equilibration time of a bulk melt.

In this talk, after introducing the physics behind the mechanisms of irreversible adsorption, I shall review some of these observations, focusing on those related to the thermal glass transition and to the segmental dynamics. Based on the information collected on different polymers, I will discuss on different models that could explain the origin of the striking correlation between the value of the glass transition temperature of 1D confined polymers and the degree of adsorption.

After presenting new results on the interplay between segmental dynamics and formation of adsorbed layers, I will demonstrate that, differently than what currently speculated, the transformation materials undergo during adsorption does not mimic physical aging.

CPP 22.8 Tue 11:45 ZEU 250

Polymer films deposited on solid surfaces studied with mesoscopic and microscopic models — Jianguo Zhang, Debashish Mukherji, Kurt Kremer, and •Kostas Daoulas — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Polymer films deposited on solid substrates are interesting for basic polymer physics and have numerous industrial applications. Here, to study these systems, we develop [1] a special particle-based model where polymers are represented as worm-like chains, while non-bonded interactions are defined [2] via a simple density functional. To specify the functional and the associated parameters, certain thermodynamic properties known from experiments are taken into account. Films of poly(methyl methacrylate) adsorbed onto silica surfaces are chosen as test cases. To validate the mesoscopic model we perform a direct comparison with smaller scale simulations, based on a generic microscopic model representing the same system. The comparison is performed considering observables such as chain-shape, structure of adsorbed layer, statistics of loops, tails, and trains. The two models are found to be consistent with each other. Certain deviations in polymer conformations and structure of adsorbed layer can be rationalized by the simplified description of polymer-surface interactions and liquid structure in the mesoscale model. [1] Zhang et al, EPJ SP 2016. [2] Daoulas and Müller, JCP 2006.

CPP 22.9 Tue 12:00 ZEU 250

EMC: A monte carlo scheme with energyconservation applied to a soft, coarse-grained model of polymers — •Marcel Langenberg — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Deutschland

Coarse-graining reduces the number of degrees of freedom (DoF) and the integrated out DoF gives rise to friction and noise and the coarse-grained beads are endowed with an internal energy. We derive the universal form of the internal energy-entropy relation in the limit of large molecular weight. Motivated by the idea of eDPD we developed an energy Monte-Carlo scheme, which locally conserves energy and momentum and does not suffer from discretization errors [1]. This simulation technique allows us to study thermal transport in diblock copolymer nanocomposites. Our coarse-grained model captures the difference between inter- and intramolecular transport and can address large Lewis numbers, which are characteristic for polymers. We investigate the Kapitza resistance of interfaces and study its dependence on the molecular architecture.

[1] M. Langenberg and M. Müller, EMC: A monte carlo scheme with energyconservation, EPL 114, 20001 (2016).

Invited Talk CPP 22.10 Tue 12:15 ZEU 250

Molecular-level framework for the dynamic mechanical response and yielding of polymer glasses — •Alessio Zaccone[1], Vladimir Palyulin[1], Chris Ness[1], Robert Elder[2], Rico Milkus[1], and Timothy Sirk[2] — [1]University of Cambridge, UK — [2]US Army Research Laboratory, USA

Understanding the mechanical response of polymer glasses is currently one of the biggest challenges in polymer physics and soft matter. The deformation of polymer glasses has a considerable non-affine component at the monomer-unit level, meaning that every unit within every chain undergoes an additional displacement on top of the displacement imposed by the strain tensor [1]. We used theoretical and computational approaches, based on the non-affine molecular-level dynamics and on the vibrational density of states. A mechanistic assessment is obtained of how chemistry-dependent many-body angular constraints along the chain and cross-linking constraints affect: 1. the value of Tg (as parameterized also by the critical number of total nearest-neighbour units at the transition, z* [2]), 2. the rate-dependent elasticity/rigidity component of response, 3. the rate-dependent energy-absorption and ductility, and 4. the yielding transition [3]. This theoretical description poses the basis of a new chemical-design platform for linking polymer chemistry to mechanical performance in advanced polymer-based functional materials. [1] A. Zaccone & E.M. Terentjev, Phys. Rev. Lett. (2013). [2] A. Lappala, A. Zaccone, E.M. Terentjev, Soft Matter (2016). [3] V. Palyulin, C.J. Ness, R. Milkus, R. Elder, T. Sirk, A. Zaccone, in preparation.

CPP 23: Organic Semiconductors (joint session CPP/DS/HL, organized by HL)

Time: Tuesday 9:30–13:15 Location: POT 251

CPP 23.1 Tue 9:30 POT 251

Femtosecond time-resolved spectroscopy of an acceptor-donor-acceptor oligomer film — •Ephraim Sommer[1], Antonietta De Sio[1], Elena Mena-Osteritz[2], Peter Bäuerle[2], and Christoph Lienau[1] — [1]Institut für Physik, Carl-von-Ossietzky Universität Oldenburg — [2]Institut für Organische Chemie II und Neue Materialien, Universität Ulm

Conjugated oligomers are gaining increasing popularity for application in organic solar cells as photoactive materials thanks to their high production reproducibility and device efficiencies [1]. However, a detailed understanding of the initial charge transfer in such systems is missing. Recently, in polymer based active materials it was found that coherent vibronic coupling plays an important role in this process [2]. This raises the question whether this also holds for oligomers. To answer this, we investigate a novel A-D-A-type oligomer by pump-probe and 2D electronic spectroscopy with femtosecond time resolution. Upon selective excitation of the donor unit, we observe strong peak-shifts of the exciton signals as a most dominant feature at early times. Moreover, the signal shows long lived vibrational oscillations. Such a peak shift cannot be explained within a vibronically coupled dimer model including only one dominant vibrational mode like in [2]. Our preliminary results suggest that the photoinduced charge transfer may occur via a conical intersection between the donor and acceptor potential energy surfaces. We will discuss theoretical modelling aimed at validating this idea.

[1] R. Fitzner et al., Adv. Funct. Mater., 12, (2015)

[2] A. De Sio et al., Nat. Commun., 7, (2016)

CPP 23.2 Tue 9:45 POT 251

Polariton bottleneck dynamics in organic microcavities — •Felix Lemke, Hartmut Fröb, and Karl Leo — IAPP, TU Dresden, Germany

Organic molecules are known to be promising candidates for strong coupling experiments due to their large exciton binding energy. Simultaneously, organic materials reveal large inhomogeneously broadened absorption spectra, complicating the investigation. Even so, small organic molecules have advantages in processing, stability (to ambient conditions and high optical excitation) and lifetime.

In this work we will present a method to investigate the microcavity polariton properties utilizing the oligomer Bu4-Ph4-DIP. We perform angle-resolved streak camera measurements and compare the data with a rate-equation model. Simulation and measurement agree very well. From this, we can see directly the influence of the polariton bottleneck, which proofs, that our system is in the strong coupling regime. Moreover, we can extract the characteristic time constants and gain an insight into the polariton dynamics.

CPP 23.3 Tue 10:00 POT 251

Charge-exciton quenching in organic transistors — •Wouter Koopman[1,2], Stefano Toffanin[2], and Michele Muccini[2] — [1]Universität Potsdam, Potsdam, Deutschland — [2]CNR-ISMN, Bologna, Italien

Organic Light-Emitting Transistors (OLETs) possess a huge potential for the design of highly integrated multifunctional optoelectronic systems and intense nanoscale light sources, such as the long-searched-for electrically pumped organic laser. In order to fulfill these promises, the efficiency and brightness of the current state-of-the-art devices have to be increased. The dominating quenching process limiting the external quantum efficiency in OLETs is charge-exciton interaction. A comprehensive understanding of this quenching process is therefore of paramount importance. The present talk reports a systematic investigation of charge-exciton interaction in organic transistors employing time-resolved photoluminescence electro-modulation (PLEM) spectroscopy on the picosecond timescale. The results show that the injected charges reduce the exciton radiative recombination in two ways: (i) charges may prevent the generation of excitons and (ii) charges activate a further non-radiative channel for the exciton decay. Moreover, the transient PLEM measurements clearly reveal that not only trapped charges, as it is was already reported in literature, but rather the entire injected charge density contributes to the quenching of the exciton population. Finally, lessons for the design of high-efficiency OLET are disused.

CPP 23.4 Tue 10:15 POT 251

Investigating the doping efficiency of organic semiconductors by thermoelectric measurements — •Bernhard Nell[1], Markus Krammer[2], Karin Zojer[2], and Koen Vandewal[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials, Technische Universität Dresden, Dresden, Germany — [2]Institute of Solid State Physics, Technische Universität Graz, Graz, Austria

We use thermovoltage (Seebeck effect) and temperature-dependent conductivity measurements on doped organic semiconductors to determine the dominating type of charge carriers introduced by the dopant and to gain insight into the position of the transport level with respect to the Fermi level. The investigation of fullerene dopants with a high degree of fluorination in various amorphous host materials allows us to tune the energy level offset between host and dopant and to study their influence on Fermi level position and overall doping efficiency systematically. Combining thermoelectric measurements with Kinetic Monte Carlo simulations gives further insight into the influence of Coulomb interactions on the trapping of mobile charge carriers in doped organic semiconductors. We find that at low doping concentrations a high amount of charge carriers is immobilized in trap states, leading to a reduced doping efficiency. Upon increasing the doping concentration, the trap states are subsequently passivated and an increased doping efficiency can be observed. Furthermore the doping efficiency is increased upon fluorination of the dopant molecules and we find a correlation between the energy level offset and the doping efficiency, at the same molar concentration.

CPP 23.5 Tue 10:30 POT 251

Vibronic coherence in a reference organic photovoltaic blend — •Antonietta De Sio[1], Ephraim Sommer[1], James Lim[2], Susana F. Huelga[2], Martin B. Plenio[2], Giulio Cerullo[3], and Christoph Lienau[1] — [1]Institut für Physik, Universität Oldenburg, Germany — [2]Institut für Theoretische Physik, Universität Ulm, Germany — [3]Department of Physics, Politecnico di Milano, Italy

The microscopic mechanisms underlying charge separation in organic solar cells are still highly debated. Although recent theoretical work [1] suggests that vibronic couplings may lie at the origin of efficient charge generation in such systems, clear experimental evidence on the role of vibronic coherence for charge separation is still lacking. Here we use ultrafast two-dimensional electronic spectroscopy with 10-fs time resolution to investigate the initial dynamics of excitons and polaronic species in P3HT and P3HT:PCBM thin films with different acceptor concentration. Our experimental results, supported by theoretical simulations, show that strong vibronic coupling favors exciton delocalization and accelerates charge separation even in presence of disorder, resulting in long-lived coherent oscillatory dynamics of strongly correlated excitons and polaron pair states, mutually coupled to a dominant vibrational mode. These results allow us to gain fundamental new insights into the initial dynamics of charge separation and may open up new perspectives for optimizing devices [2,3].

[1] Tamura et al, JCP 137, 22A540, 2012. [2] Falke et al, Science 344, 1001, 2014. [3] De Sio et al, Nat.Commun. 2016 in press.

CPP 23.6 Tue 10:45 POT 251

Crystalline Packing Motifs in Pentacene-like Organic Semiconductors — •Michael Klues and Gregor Witte — Fachbereich Physik, Universität Marburg, Germany

While the impact of chemical modifications on the molecular electronic system can be well computed, the influence on solid state properties is hardly predictable. In fact already slight chemical modifications, like the introduction of heteroatoms or small side groups, often lead to dramatically changed crystal structures and thereby rather different charge carrier mobilities or exciton binding energies. Within a comparative study of various pentacene-like organic semiconductors, based on a Hirshfeld analysis [1] we reveal correlations between molecular properties and packing motives. By choosing molecules with nearly identical geometrical dimensions the complexity of intermolecular interactions is considerably reduced and effects of electrostatic potentials, hydrogen bonds and atom sizes can be carved out. Thereby, we attain a simple rule for predicting the occurrence of herringbone packing motifs and point out the relevance of hydrogen bonds for parallel molecular arrangements as found previously for partially fluorinated HBC. [2] Furthermore we suggest a route to increase intermolecular orbital overlap by integration of large heteroatoms in the periphery of aromatic systems which yields an improved charge carrier mobility in the case of DNTT.

[1] M.A Spackman; D. Jayatilaka, CrystEngComm, 11, 19, (2009)

[2] T. Breuer et al., Phys. Chem. Chem. Phys., (2016), DOI: 10.1039/C6CP06126E

Coffee Break

CPP 23.7 Tue 11:30 POT 251

Strongly reduced inhomogeneous broadening of molecular aggregates in hybrid nanostructure system — •Xuan Trung Nguyen[1], Antonietta De Sio[1], James Lim[2], Alexandra Markovic[3], Julia Witt[3], Gunther Wittstock[3], Susana Huelga[2], Martin Plenio[2], and Christoph Lienau[1] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany — [2]Institut für Theoretische Physik and IQST, Universität Ulm, Germany — [3]Institut für Chemie, Carl von Ossietzky Universität Oldenburg, Germany

The applications of nanostructures based on organic molecular aggregates range from solar cells to all-optical switching. These aggregates are often modeled as disordered systems that exhibit inhomogeneously broadened absorptive line shapes. In such a system, disorder localizes the exciton wavefunction and leads to limited exciton transport efficiency, which is important in devices like solar cells. By using linear and non-linear spectroscopy, we show that the inhomogeneous broadening of a model J-aggregate cyanine dye is strongly reduced in the presence of an ultrathin gold layer and the resulting optical spectra display almost perfect Lorentzian line shapes. Supported by theoretical simulations, we explain the experimental results in terms of increased delocalization of the exciton wavefunction due to electronic coupling to surface plasmon polaritons supported by the aggregate-gold. This coupling can average out the disorder effect and thus increase the exciton transport efficiency.

CPP 23.8 Tue 11:45 POT 251

The Influence of Molecular Packing on Charge-Transfer States at the Pentacene/Perfluoropentacene Interface — •Andre Rinn[1], Tobias Breuer[1], Julia Wiegand[2], Michael Beck[2], Jens Hübner[2], Michael Oestreich[2], Gregor Witte[1], and Sangam Chatterjee[3] — [1]Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, D-30167 Hannover, Germany — [3]Institute of Experimental Physics I, Justus-Liebig University Giessen, Heinrich-Buff-Ring 16, D-35392 Gießen, Germany

We study different model systems of intermixed and layered heterostructures of pentacene and perfluoropentacene by means of time resolved photoluminescence spectroscopy to investigate the impact of molecular packing at the interface on the optical properties. We assign the different PL signals visible in the heterostructures to their respective origin and find an increase in the PL intensity of the charge-transfer signal for pi-stacking at the interface. Significantly slower carrier dynamics are measured for the charge-transfer states when compared to bulk exciton emission which are quenched by singlet exciton fission.

CPP 23.9 Tue 12:00 POT 251

Three-dimensional confinement and exciton-polaritons in open organic microcavities — •Simon Betzold[1], Marco Dusel[1], Jürgen Ohmer[2], Utz Fischer[2], Christof P. Dietrich[1], and Sven Höfling[1,3] — [1]Technische Physik, Universität Würzburg — [2]Institut für Biochemie, Universität Würzburg — [3]SUPA, School of Physics and Astronomy, University of St Andrews

Frenkel excitons, characteristic of organic semiconductors, possess large binding energies making them stable at room temperature, rendering polariton experiments at ambient air conditions possible. Organic materials further exhibit very large oscillator strengths and thus strongly interact with a cavity field. Since organic materials are very sensitive to the deposition of semiconductor layers on top of them, we use an open cavity system, which makes non-invasive investigation possible. Open cavities are tunable systems and comprise a bottom semiconductor distributed Bragg reflector (DBR) with the active material (the organic semiconductor) on top and a concave top DBR separated by a micrometer sized air gap. This configuration allows a 3D photonic confinement and brings unprecedently high quality factors into reach.Here, we show the versatility of open cavities by performing reflectivity and photoluminescence measurements in Fourier imaging configuration and exemplary investigate the strong exciton-photon coupling between a fluorescent protein and the dielectric cavity. We emphasize that the open cavity approach can easily be extended to more complex systems like photonic lattices and active regions including 2D monolayer materials or hybrid organic-inorganic bilayers.

CPP 23.10 Tue 12:15 POT 251

Improving lasing properties of a hybrid OLED/microcavity structure — •Stefan Meister, Robert Brückner, Markas Sudzius, Hartmut Fröb, and Karl Leo — IAPP, TU Dresden, Germany

Organic materials have many advantages which can be utilized in different kinds of devices such as light-emitting diodes, solar cells, or even lasers. Some examples are the spectrally separated broad absorption and emission spectra, the possibility to build very thin and flexible devices, and the fact of having an intrinsic four-energy-level-system.

The goal of realizing an electrically driven organic solid state laser is so far well beyond reach. As a first step, we incorporate an OLED into a microcavity (MC) consisting of two Distributed Bragg Reflectors (DBR). These devices are investigated electrically and with a micro-photoluminescence setup to determine the optical functionality. The optical measurements further allow to compare it to standard organic MCs. These insights are analyzed and addressed with the help of photolitography to improve the quality of the metal layers. Further, different very thin (60nm - 0.15mm) encapsulation methods are tested to allow measurements under ambient conditions.

CPP 23.11 Tue 12:30 POT 251

High temperature stable single carrier hole only devices — •Shahidul Alam[1,2], Peter Fischer[3], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Center for Energy and Environmental Chemistry Jena (CEEC Jena) Friedrich-Schiller-Universität Jena Philosophenweg 7a 07743 Jena, Germany — [2]Institute of Organic and Macromolecular Chemistry Friedrich-Schiller-Universität Jena Humboldtstr. 10 07743 Jena, Germany — [3]Institut für Werkstofftechnik, TU Ilmenau, Gustav-Kirchhoff-Str. 6, 98693 Ilmenau, Germany

Thin hole transport layers (HTL) are crucial elements in organic semiconductor based devices. Metal oxides are an encouraging material class for this purpose. Metal oxides can be used to modify either of the two contacts in a device for improved wettability as well as chemical and electronic compatibility of the contacts with the organic layer. Several materials like NiO, V2O5, WO3 and MoO3 have demonstrated encouraging prospective for performing as efficient charge transport layers. Among them molybdenum oxide (MoO3) attracted extensive interest due to its superior performance. In order to evaluate charge transport properties of annealed semiconductor films, devices are required to be stable at high annealing temperature. Whereas PEDOT:PSS has generally proper charge injection and extraction properties, these may drastically change upon heating above certain temperature. In this work, we show that a MoO3 interlayer can efficiently substitute PEDOT:PSS as hole transport layer within single carrier hole only devices (SCHD), because of its better stability at high annealing temperature.

CPP 23.12 Tue 12:45 POT 251

Tuning the conductivity in organic-based charge-transfer materials: A combined NEXAFS and electrical transport study — •Antonia Morherr[1], Sebastian Witt[1], Alisa Chernenkaya[2], Katja Medjanik[2], Gerd Schönhense[2], Harald O. Jeschke[3], Roser Valentí[3], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe Universität, 60438 Frankfurt am Main — [2]Institut für Physik, Johannes Gutenberg-Universität, 55099 Mainz — [3]Institut für theoretische Physik, Goethe Universität, 60438 Frankfurt am Main

Single crystals of the novel charge transfer complexes phenanthrene- and picene/TCNQ-F$_x$ (x=0,2,4) were grown by physical vapor transport [1] and investigated by electrical transport measurements, near-edge X-ray absorption spectroscopy (NEXAFS) and density functional theory calculations. The electrical conductivity and the mobility of the samples increase with increasing acceptor strength. The activation energy of the complexes was studied by temperature dependent measurements and compared to the electrical band structure investigated by NEXAFS [2]. The results were compared to the DFT calculations for the electrical band structure and simulated NEXAFS spectra.

[1] A. Morherr et al., Physica B 496, 98-105 (2016)

[2] A. Chernenkaya et al., J. Chem. Phys. 145, 034702 (2016)

CPP 23.13 Tue 13:00 POT 251

Three-dimensional photonic confinement of imprinted pillars in an organic Tamm-plasmon structure — •Marco Dusel[1], Simon Betzold[1], Christof P. Dietrich[1] und Sven Höfling[1,2] — [1]Technische Physik, Julius-Maximilians-Unversität Würzburg, Am Hubland, 97074 Würzburg — [2]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, UK

The fluorescence of organic solids at room temperature is governed by the radiative decay of Frenkel excitons that are characterized by large exciton binding energies and short Bohr radii compared to inorganic semiconductors. Due to their very large oscillator strength, organic materials further strongly interact with light, in particular in microcavities.

So far, photonic confinement within the cavity plane has mainly been achieved by tailoring the dielectric part of the cavity. Here, we present a novel technology that enables 3D photonic confinement within the active organic layer of a Tamm-plasmon structure (metal-clad cavity) by laterally imprinting pillars. The fabricated pillars have diameters ranging from 7 to 20 μm and heights between 2 and 4 μm. The developed technology enables far more complicated photonic potentials including coupled pillars, chains and lattices.

CPP 24: Colloids and Complex Fluids I (joint session BP/CPP/DY, organized by CPP)

Time: Tuesday 11:30–13:00 Location: ZEU 255

CPP 24.1 Tue 11:30 ZEU 255

Small activity differences drive phase separation in polymers — •Jan Smrek and Kurt Kremer — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Recent theoretical studies found that mixtures of active and passive colloidal particles phase separate but only at very high activity ratio. The high value poses serious obstacles for experimental exploration of this phenomenon. Here we show using simulations that when the active and passive particles are *polymers*, the critical activity ratio decreases with the polymer length. This not only facilitates the experiments but also has implications on the DNA organization in living cell nuclei. Entropy production can be used as an accurate indicator of this non-equilibrium phase transition.

CPP 24.2 Tue 11:45 ZEU 255

Corresponding States Law For Protein Solutions — •Florian Platten and Stefan U. Egelhaaf — Heinrich Heine University, Condensed Matter Physics Laboratory, Duesseldorf, Germany

The extended law of corresponding states, as proposed by Noro and Frenkel, involves a mapping of the phase behavior of systems with short-ranged attractions. We test its applicability to protein solutions with their complex interactions. We successfully map the experimentally determined metastable gas-liquid binodals to the binodals of short-ranged square-well fluids. This is achieved by representing the binodals as a function of the temperature scaled with the critical temperature (or as a function of the reduced second virial coefficient) and the concentration scaled by the cube of an effective particle diameter, where the scalings take into account the attractive and repulsive contributions to the interaction potential, respectively. The scaled binodals of the protein solutions coincide with simulation data of the adhesive hard-sphere fluid. Furthermore, once the repulsive contributions are taken into account by the effective particle diameter, the temperature dependence of the reduced second virial coefficients follows a master curve that corresponds to a linear temperature dependence of the depth of the square-well potential. We moreover demonstrate that, based on this approach and cloud-point measurements only, second virial coefficients can be estimated, which we show to agree with values determined by light scattering or by Derjaguin-Landau-Verwey-Overbeek (DLVO)-based calculations.

Platten et al., J. Chem. Phys. 142, 174905 (2015).

CPP 24.3 Tue 12:00 ZEU 255

Critical Casimir interactions between Janus particles — •Marcel Labbé-Laurent and Siegfried Dietrich — Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany

Critical fluctuations in binary liquid mixtures give rise to forces acting on immersed colloidal particles. Experiments have demonstrated a remarkable agreement with theoretical predictions for spherical colloids close to a (chemically patterned) substrate [1,2]. At the same time, there has been strong experimental and theoretical interest in studying the self-assembly and the phase behavior of patchy and Janus particles. Although a variety of effective interactions have been proposed to drive the self-assembly, the critical Casimir effect stands out as being particularly suitable because it provides both attractive and repulsive interactions depending on the chemical surface properties, as well as a sensitive control of their strength via minute temperature changes. We present theoretical calculations for the interaction between a single Janus particle and a chemically structured substrate and the effective pair potential between two Janus cylinders as well as between two Janus spheres [3].

[1] C. Hertlein, L. Helden, A. Gambassi, S. Dietrich, and C. Bechinger, *Nature* **451**, 172 (2008).

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

[3] M. Labbé-Laurent, and S. Dietrich, *Soft Matter* **12**, 6621 (2016).

CPP 24.4 Tue 12:15 ZEU 255

From criticality to gelation in sticky spheres — David Richard[1,2], Thomas Speck[1], and •Cristopher Patrick Royall[2] — [1]Institut fur Physik, Johannes Gutenberg-Universitat, Mainz, Germany — [2]HH Wills Physics Laboratory, Tyndall Avenue, Brisol, United Kingdom

Understanding the mechanism of dynamical arrest in liquids is a long standing challenge. Even for simple fluids, such as sticky spheres, an arrested gel can occur when the system is quenched sufficiently fast such that it cannot relax to equilibrium. For many systems the gelation arises at the gas-liquid phase boundary, forming a rigid but dilute network of bonded particles. In this study, we look at the critical behavior of sticky spheres combining confocal microscopy of colloid-polymer mixtures and Monte Carlo simulations of the square-well model. The mapping between those two is achieved via tracking colloids at the single-particle level and fitting pair distribution functions to the simulation data. We then compare the local structure via the topological cluster classification (TCC) method to identify locally favored structures (LFSs) along the critical path. We observe a very good agreement between experiments and simulations, where the growth of highly ordered structures are triggered even far away from the phase boundary. We discuss the link of those LFSs to the global percolating bond network.

CPP 24.5 Tue 12:30 ZEU 255

Determination of crystal nucleation barriers for colloidal crystals from computer simulations — •Peter Koss[1,2], Antonia Statt[3], Peter Virnau[1], and Kurt Binder[1] — [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 — [3]Princeton University, Princeton, NJ 08544, USA

A fluid in equilibrium, confined in a finite volume, with a density exceeding the onset of freezing, may exhibit phase coexistence with a crystal nucleus surrounded by liquid or a gas. Classical nucleation theory predicts that the barrier of homogeneous nucleation is given by two contributions, the free energy gained by the creation of a crystal droplet and the free energy loss due to surface tension of the newly created interface. We obtain the excess free energy due to the surface of the crystalline nucleus by using a computational method suitable for the estimation of the chemical potential of dense fluids. Our analysis method is appropriate for crystal nuclei of all shapes, without suffering from ambiguities occurring when one needs a microscopic identification of the crystalline droplet. We present a novel analysis method to determine the coexistence pressure between fluid and crystal, and report that the nucleation barrier for a soft version of the effective Asakura-Oosawa model is compatible with a spherical shape, and consistent with classical nucleation theory [1].

[1] A. Statt, P. Virnau, and K. Binder, Phys. Rev. Lett. 114, 026101 (2015).

CPP 24.6 Tue 12:45 ZEU 255

Phonons and Elasticity in Disordered binary Crystals — •Tadeus Ras and Matthias Fuchs — FB Physik, Univ. Konstanz

The "method of long waves" is a well-established tool for the study of elastic constants [1]. However, until recently, it had been lacking in crystals with point defects due to an unclear definition of the displacement field.

We present a generalization of the projection-operator approach employed in [2]. It yields expressions for the elastic constants valid in binary crystals with arbitrary amounts of point defects and up to the melting temperature. Further, both acoustic and optical phonon eigenfrequencies can be computed in linear response.

While density functionals from classical DFT serve as an input parameter to the approach it can also be employed experimentally to process measurement data. For demonstration, dispersion relations will be shown as obtained from molecular dynamics data of a hard sphere model crystal [3].

[1] D. C. Wallace, Thermodynamics of Crystals (Wiley, NY 1972).

[2] C. Walz and M. Fuchs, Phys. Rev. B **81**, 134110 (2010).

[3] L. Filion et. al., Phys. Rev. Lett. **107**, 168302 (2011).

CPP 25: Fundamentals of Perovskite Photovoltaics IV (joint session CPP/DS/HL)

Time: Tuesday 14:00–16:00 Location: ZEU 222

Invited Talk CPP 25.1 Tue 14:00 ZEU 222

Ultrafast transient absorption spectroscopy of organic-inorganic hybrid perovskites on mesoporous titanium dioxide in contact with hole transport materials — •Thomas Lenzer — Universität Siegen, Physikalische Chemie, Adolf-Reichwein-Str. 2, 57076 Siegen

Organic-inorganic hybrid perovskites, such as methylammonium lead iodide, are particularly promising for applications in solar light harvesting and optoelectronics. We present our recent results on the carrier dynamics of such materials using ultrafast pump - supercontinuum probe spectroscopy in the 260-1600 nm range. The perovskite systems are investigated over a wide range of carrier densities. Slow carrier recombination processes, ”phonon bottlenecks” during carrier cooling and confinement effects in low-dimensional perovskite structures are identified. We investigate electron injection processes from the perovskite into the mesoporous titania scaffold and estimate the relative contributions of electron transport pathways in the perovskite and titanium dioxide. We also discuss the hole transfer from the perovskite into triarylamine-based hole transport materials (HTMs).

CPP 25.2 Tue 14:30 ZEU 222

Identification of charge transport limiting factors in perovskite-based solar cells by Time-of-Flight measurements — •Irene Grill^{1,2}, Meltem Aygüler^{1,2}, Nadja Giesbrecht^{1,2}, Pablo Docampo^{1,2}, Thomas Bein^{1,2}, Matthias Handloser^{3}, and Achim Hartschuh^{1,2} — ^{1}Department of Chemistry & CeNS, LMU Munich — ^{2}Nanosystems Initiative Munich (NIM) — ^{3}Toptica Photonics AG

Hybrid perovskites represent one of the most promising absorber materials for future photovoltaic applications due to the recently achieved high PCE values [1]. In this work, we determine the transport time of photoinduced charges in between the top- and bottom-electrode in perovskite thin film solar cells upon pulsed laser excitation, using Time-of-Flight (ToF) photocurrent measurements. To extract the influence of the individual layers on the transport characteristics and to identify limiting factors we carried out additional ToF studies on the respective absorber layer of the photovoltaic device in a lateral architecture. The results of the single film measurements are discussed in terms of crystal size and orientation. The direct comparison of the data obtained for the individual layers and the photocurrent transients of the final device under working conditions permits the identification of limiting factors for inter-facial and intra-film charge transport simultaneously to allow for the optimization of both the fabrication techniques [2,3] and device architecture. [1] M. Saliba et al., Energy Environ. Sci. 2016, 9, 1989. [2] I. Grill et al., Sol. Energ. Mat. Sol. Cells 2016, accepted. [3] A. Binek, I. Grill et al., Chem. Asian J. 2016, 11, 1199.

CPP 25.3 Tue 14:45 ZEU 222

Fill factor optimization strategies in efficient, stable triple cation perovskite solar cells — •Martin Stolterfoht, Christian Wolff, Yochai Amir, Andreas Paulke, and Dieter Neher — Institute of Physics and Astronomy, University of Potsdam, Potsdam-Golm, Germany

Perovskite solar cells (PSCs) now compete with their inorganic counterparts in terms of power conversion efficiency. To advance this technology even further, more insights into the physical mechanisms that define the bias dependence of the photocurrent are required. In this work, we varied the organic electron/hole transport layers (ETL/HTL) thickness in efficient triple cation PSCs and studied the charge carrier recombination and transit through the device. Using resistance dependent photovoltage (RPV), we identify the transit time through the transport layers as key figure of merit for maximizing the fill factor (FF) and the overall photovoltaic performance. The results are complemented by intensity dependent photocurrent measurements which elucidate the role of the HTL thickness on the bias dependence of the recombination losses and recombination order. By optimizing the transit time through the HTL (undoped PTAA) we demonstrate efficiencies under solar AM1.5G conditions of up to 20.4% with high FFs of 80%. The reported cells also exhibit excellent stability under light illumination and stability in air, even without encapsulation. However, further improving the FF via a continuous reduction of the HTL leads to significant open-circuit voltage losses which highlights the challenge to simultaneously optimize the FF and open-circuit voltage.

CPP 25.4 Tue 15:00 ZEU 222

Optical phonons in methylammonium lead halide perovskites and implications for charge transport — •Michael Sendner^{1,2}, Pabitra K. Nayak^{3}, David A. Egger^{4}, Sebastian Beck^{1,2}, Christian Müller^{1,2,5}, Bernd Epding^{2,5}, Wolfgang Kowalsky^{1,2,5}, Leeor Kronik^{4}, Henry J. Snaith^{3}, Annemarie Pucci^{1,2}, and Robert Lovrincic^{2,5} — ^{1}Kirchhoff-Institut für Physik, Universität Heidelberg — ^{2}InnovationLab, Heidelberg — ^{3}Clarendon Laboratory, University of Oxford — ^{4}Department of Materials and Interfaces, Weizmann Institute of Science — ^{5}Institut für Hochfrequenztechnik, TU Braunschweig

Recent reports indicated that the mechanical and electronic properties of lead-halide perovskites are strongly affected by the lattice vibrations. Herein we report far-infrared spectroscopy measurements of $CH_3NH_3Pb(I/Br/Cl)_3$ thin films and single crystals at room temperature (RT) and a detailed quantitative analysis of the spectra. We find strong broadening and anharmonicity of the lattice vibrations for all three halide perovskites, which indicates dynamic disorder of the lead-halide cage at RT. We determine the frequencies of the transversal and longitudinal optical phonons, and use them to calculate, via appropriate models, the static dielectric constants, polaron masses, electron-phonon coupling constants, and upper limits for the phonon-scattering limited charge carrier mobilities. Within the limitations of the model used, we can place an upper limit of 200 $cm^2V^{-1}s^{-1}$ for the RT charge carrier mobility in $MAPbI_3$ single crystals.
See also: Sendner et al., Materials Horizons, 3, pp 613-620, 2016.

CPP 25.5 Tue 15:15 ZEU 222

Advances in Vapour Deposition of Metal-Halide Perovskite Thin-Films for Solar Cells — •Juliane Borchert, Jay B. Patel, Henry J. Snaith, and Michael B. Johnston — Department of Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford, OX13PU, UK

Hybrid metal-halide perovskite materials are promising absorber materials both for use in single junction and tandem solar cells. A particular focus in recent research has been on the fabrication of perovskite absorber layers from solution. Alternatively, perovskite thin-films can also be deposited using co-evaporation in vacuum. This method offers several benefits. The obtained films show high uniformity over large surface areas. Thus the technique is well suited to the fabrication of large-area planar heterojunction solar cells. Additionally, the uniform film thickness makes the evaporated films ideal for precision characterisation of the optical properties of metal halide perovskite materials. Furthermore, the vapour deposition is solvent-free, which makes it compatible with a wide range of substrates and interlayers. This is for example advantageous in the fabrication of tandem solar cells. Here we present current advances in the understanding of the influence that different process variables have on the quality of the obtained films, as well as the application of co-evaporated perovskite absorber layers in devices.

CPP 25.6 Tue 15:30 ZEU 222

Carrier Recombination Analysis in Perovskites Using Time-Resolved Photoluminescence — •Liudmila Kudriashova^{1}, Philipp Rieder^{1}, Kristofer Tvingstedt^{1}, Andreas Sperlich^{1}, Georgy Astakhov^{1}, Andreas Baumann^{2}, and Vladimir Dyakonov^{1,2} — ^{1}Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ^{2}Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Despite the incredible progress of perovskite-based photovoltaics, many aspects of charge carrier recombination in organometal halide perovskites still remain unclear, inhibiting the targeted production of high-performance solar cells. Under solar cell operating conditions photoluminescence (PL) in perovskites is mainly caused by recombination of free photogenerated charge carriers. Hence the time-resolved photoluminescence (TRPL) is a powerful tool to reveal the complex charge carrier behaviour in perovskite films. Here, we implement the combination of several kinetic models for TRPL in $CH_3NH_3PbI_3$ and $CH_3NH_3PbI_{3-x}Cl_x$ films to extract the characteristic recombination rates and estimate the trap concentration. We obtain trap densities in the range of $10^{15} - 10^{16}$ cm^{-3} and show that PL decay drastically depends on interfaces between the perovskite and conducting layers. Currently controversial aspects, such as different recombination pathways, origin of trap states, and the effect of photon recycling, are discussed. In summary, TRPL analysis enables the calculation of trap density and clarifies the origin of defects, which is crucial for the further development of perovskite-based photovoltaics.

CPP 25.7 Tue 15:45 ZEU 222

Monolithic serial interconnection of perovskite solar cells using laser ablation — •Felix Schneider[1], Christof Schultz[1], Rutger Schlatmann[1,2], Steve Albrecht[3], and Bert Stegemann[1] — [1]HTW Berlin - University of Applied Sciences, Wilhelminenhofstr. 75a, 12459 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, PVcomB, Schwarzschildstr. 3, 12489 Berlin, Germany — [3]Helmholtz-Zentrum Berlin, Institut für Silizium-Photovoltaik, Kekuléstraße 5, 12489 Berlin, Germany

Based on recent work on serial interconnection of thin film solar cells by laser ablation, the proper laser parameters for scribing planar, inverted perovskite solar cell samples were determined. A device design with the layer sequence ITO/PTAA/perovskite/PCBM/Ag was used in which the P1 scribes the ITO, the P2 separates the perovskite and the selective contact layers and the P3 the metal electrode. As a result, successful P1 to P3 laser scribes with sufficiently small area losses, i.e. small dead areas, were obtained. Degradation due to humidity of the perovskite layer during laser scribing was avoided by complete laser processing in nitrogen atmosphere. Detailed characterization of the sample composition by energy dispersive x-ray spectroscopy, the morphology by atomic force microscopy as well as of the electrical functionality of the P2 scribes will be provided. The influence of laser-induced material modifications in the vicinity of the laser scribes on the module performance will be discussed.

CPP 26: Molecular Electronics and Excited State Properties

Time: Tuesday 14:00–16:00 Location: ZEU 260

CPP 26.1 Tue 14:00 ZEU 260

Ultrafast Exciton Dynamics in Diindenoperylene Films — •Marc Hänsel[1], Valentina Belova[2], Katharina Broch[2], Frank Schreiber[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg, Germany — [2]Institut für Angewandte Physik, Universität Tübingen, Germany

Diindenoperylene (DIP) is a very promising material for organic electronics. It shows a high charge-carrier mobility, forms thin films with high structural order and is resistant to most environmental influences. In a photovoltaic device it can be used as donor or acceptor material. In this work we monitored the ultrafast (sub picosecond) excited states dynamics in DIP after optical excitation using time-resolved second harmonic generation (TR-SHG). We investigated the exciton dynamics in thin DIP films on two different substrates, namely SiO2 and Sapphire. Sapphire was used as non-interacting substrate to analyze the behavior of excitonic species in the pure DIP film. The generation dynamics of singlet excitons localized on single molecules followed by the formation of charge transfer excitons between two DIP molecules could be resolved. On the SiO2 (native oxide layer 2nm) additional ultrafast processes were found, due to electronic coupling effects between DIP and the semiconducting substrate.

CPP 26.2 Tue 14:15 ZEU 260

Tuning nonradiative lifetimes via molecular aggregation — •Alan Celestino and Alexander Eisfeld — MPIPKS, Dresden, Germany

We show that molecular aggregation can strongly influence the nonradiative decay (NRD) lifetime of an electronic excitation. As a demonstrative example, we consider a transition-dipole-dipole-interacting dimer whose monomers have harmonic potential energy surfaces (PESs). Depending on the position of the NRD channel ($q_{\rm nr}$), we find that the NRD lifetime ($\tau_{\rm nr}^{\rm dim}$) can exhibit a completely different dependence on the intermolecular-interaction strength. We observe that (i) for $q_{\rm nr}$ near the Franck-Condon region, $\tau_{\rm nr}^{\rm dim}$ increases with the interaction strength; (ii) for $q_{\rm nr}$ near the minimum of the monomer excited PES, the intermolecular interaction has little influence on $\tau_{\rm nr}^{\rm dim}$; (iii) for $q_{\rm nr}$ near the classical turning point of the monomer nuclear dynamics, on the other side of the minimum, $\tau_{\rm nr}^{\rm dim}$ decreases with the interaction strength.

[1] arXiv:1611.09115 [physics.chem-ph]

CPP 26.3 Tue 14:30 ZEU 260

Effective Treatment of Quantum Dissipation at a Conical Intersection — •Hong-Guang Duan[1,2,3], R. J. Dwayne Miller[1,3,4], and Michael Thorwart[2,3] — [1]Max-Planck Institute, Hamburg, Germany — [2]Univerisity of Hamburg, Hamburg, Germany — [3]Center for Ultrafast Imaging, Hamburg, Germany — [4]University of Toronto, Toronto, Canada

A conical intersection (CI) is a degenerate point of two potential energy surfaces (PESs) in the configuration space of a polyatomic molecule. It enables an ultrafast radiationless transition of an electronic wave packet between two PESs. Yet, revealing the details of the nonadiabatic quantum dynamics in the vicinity of a CI is still challenging because the CI usually involves an enormous number of the electronic and nuclear degrees of freedom. Advanced quantum chemistry provide an atomic view of the quantum dynamics but limited by the number of atoms. Here, we formulated a further reduced model to describe the nonadiabatic quantum dynamics around the CI. By transforming the tuning and coupling modes into the bath, we have significantly reduced the computational complexity, which allows for an efficient numerical treatment of a CI in the presence of strong vibrational relaxation. We have calculated the two-dimensional pump-probe spectra and identify the signature of the CI. Moreover, we have studied the impact of the vibrational coherence on the quantum efficiency of the transfer via a CI. We observe that more coherent wave packets show a higher quantum yield than the less coherent one. Our observations reproduce findings from a coherent control experiment.

CPP 26.4 Tue 14:45 ZEU 260

Phase modulated femtosecond spectroscopy for weakly interacting molecular aggregates — •Zengzhao Li and Alexander Eisfeld — Max-Planck-Institute for the Physics of Complex Systems, Noethnitzer St. 38, 01187 Dresden, Germany

Recent phase-modulated wave packet interferometry experiments on gases of alkaline atoms showed signals from states where multiple atoms are excited simultaneously [Bruder et al., Phys. Rev. A 92, 052412 (2015)]. To shed light on experimental observations, we not only numerically solve the Schrodinger equation for a typical minimal model of two interacting particles but also develop analytical formulas based on perturbation theory. Our results indicates that phase modulated femtosecond spectroscopy can probe weak dipole-dipole interactions of molecular aggregates.

CPP 26.5 Tue 15:00 ZEU 260

Stained microparticles for lifetime encoding — •Daniel Kage[1], Linn Fischer[1], Katrin Hoffmann[1], Marc Wittkamp[2], Jens Ameskamp[2], Wolfgang Göhde[2], Thomas Thiele[3], Uwe Schedler[3], and Ute Resch-Genger[1] — [1]Bundesanstalt für Materialforschung und -prüfung (BAM), Richard-Willstätter-Str. 11, 12489 Berlin — [2]Quantum Analysis GmbH, Mendelstr. 17, 48149 Münster — [3]PolyAn GmbH, Rudolf-Baschant-Str. 2, 13086 Berlin

Multiparametric analyses involving optical techniques like flow cytometry are at the core of studying complex systems in biological research and diagnostic applications [1]. However, for fluorescence-based techniques, the number of reporters distinguishable in spectral multiplexing is limited by spectral overlap and requires a multitude of excitation light sources and detection systems [2]. Intensity encoding often used for bead assays suffers from problems regarding dye concentration control and excitation light intensity fluctuations [2]. An alternative is luminescence lifetime encoding [3], particularly to minimize instrument costs. Here, we report on dye-stained polymer microparticles for lifetime encoding in flow cytometry with different organic dyes. This ranges from studies of the impact of parameters like dye loading concentration and particle diameter on fluorescence decay behavior to the demonstration of lifetime code reading and simultaneous ligand fluorescence signal detection with single-wavelength excitation in a flow.

[1] V. V. Tuchin, Advanced optical flow cytometry: methods and disease diagnoses. Wiley-VCH, 2011. [2] K. Hoffmann et al., ACS Nano, 2013, 7(8), 6674. [3] R. Cao et al., Opt Express, 2013, 21(12), 14816.

CPP 26.6 Tue 15:15 ZEU 260

Following a Photocatalytic Redox Cycle using Fluorescence Correlation Spectroscopy — •Josef Haimerl[1], Jan Vogelsang[1], Indrajit Ghosh[2], Burkhard König[2], and John Lupton[1] — [1]Institut für angewandte und experimentelle Physik, Universität Regensburg — [2]Institut für organische Chemie, Universität Regensburg

Rhodamine dye-based photo-induced redox catalytic processes hold great importance as efficient and, moreover, cheap alternatives to already existing transition metal-based photocatalytic processes. Recent examples show that consecutive photo-induced electron transfer processes (conPET)overcome the energetic limit of using the energy of only a single photon in photoredox catalysis. However, often, it is not clear which excited states of the photcatalysts are involved in such processes and how solvents (e.g. solvent polarity), reductants or oxidants impact the dynamics of these systems. We therefore present the use of fluorescence correlation spectroscopy (FCS) and time-correlated single photon counting(TCSPC) in order to understand the details of such photoredox catalytic processes, as well as to characterise the steps that are crucial in those photocatalytic cycles with the corresponding efficiencies .

CPP 26.7 Tue 15:30 ZEU 260

Light-Harvesting Processes Conference Revealing The Structural Properties Of Chromophores With The Help Of MD-Simulations — •Axel Bourdick and Stephan Gekle — - Biofluid Simulation and Modeling, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth, GERMANY

With the advent of organic photovoltaics promising materials for organic solar cells have become a strong focus of research. One particular interesting manufacture strategy is the push-pull chromophore design, whereby an electron rich donor unit and an electron deficient acceptor are placed alternating on the same molecule [1,2]. With the help of Molecular Dynamics Simulations we investigate the Systems p-DTS(FBTTh2)2 (T1) and p-SIDT(FBTTh2)2 (H1) [3]. We are interested in the structure and conformation of aggregated states in different solvents, and physical properties, like the free energy of the system under various conditions. By comparison with experimental results we will contribute to a better understanding of the macroscopic properties of the materials in question, which can help optimizing molecular chromophore design in future applications.

[1]*D. Gendron, M. Leclerc, (2011) Energy Environ. Sci., 4, 1225-1237

[2]*C. Duan, F. Huang, Y. Cao, (2012) J. Mater. Chem., 22, 10416-10434

[3]*J. A. Love et al., (2014), J. Am. Chem. Soc, 136(9), 3597-3606

CPP 26.8 Tue 15:45 ZEU 260

Absolute optical sensor based on biluminescence — •Caterin Salas Redondo and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials, Dresden, Germany

According to the selection rules in quantum mechanics, only transitions from the singlet excited state are allowed, deactivating radiatively while generating fluorescence emission, whereas transitions from the triplet excited state are theoretically not allowed. Nevertheless, there is a small probability of these forbidden transitions to occur at a low rate, resulting in a slow radiative deactivation known as phosphorescence emission. In this context, the property of an organic molecule able to emit photons from both their singlet and triplet excited states is called biluminescence. Although this dual state emission, particularly at room temperature, is difficult to achieve by purely organic molecules, it becomes possible if competitive non-radiative decay is suppressed effectively, allowing emission from the triplet states (i.e. phosphorescence) in addition to the conventional fluorescence. Here, we have identified biluminescence in simple host:guest systems in which a biluminophore is embedded in an optimum rigid matrix, for example, a combination of PMMA [poly(methyl methacrylate)] as host and NPB [N,N'-di(naphtha-1-yl)-N,N'-diphenyl-benzidine] as biluminophore. In this presentation, we will report on the oxygen sensing characteristics of a biluminescent system compared to a benchmarked single state optical sensor. Furthermore, we will address our efforts towards the potential integration of novel optical biluminescent sensing into organic electronics.

CPP 27: Photoswitchable Materials

Time: Tuesday 14:00–15:45 Location: ZEU 114

CPP 27.1 Tue 14:00 ZEU 114

Kinetics of light-induced ordering and deformation in LC azobenzene-containing materials — •Vladimir Toshchevikov[1], Tatiana Petrova[2], and Marina Saphiannikova[1] — [1]Leibniz-Institut für Polymerforschung, Hohe Str. 6, 01069 Dresden, Germany — [2]Cherepovets State University, pr. Lunacharskogo 5, 162600 Cherepovets, Russia

Azobenzene-containing materials are known as effective actuators of the light energy into mechanical work [1]. We develop a theory of light-induced ordering and deformation in azo-materials starting from kinetic equations of photoisomerization. The orientation interactions between rod-like trans-isomers are taken into account. Angular selectivity of the photoisomerization leads to the light-induced ordering and deformation of the azo-material. The time evolutions of ordering and deformation are found as functions of the light intensity depending on opto-mechanical characteristics of the material: probability of optical excitation of trans- and cis-isomers, angular jump during single isomerization event, viscosity of the material, strength of the orientation interactions and angular distribution of chromophores in side chains. Found structural-property relationships are in agreement with experiments and can be used for construction of light-controllable smart materials for target practical applications.

[1] Petrova T. et al., Soft Matter 11, 3412-3423, 2015.

CPP 27.2 Tue 14:15 ZEU 114

Tris(azobenzene) star: A theoretical study of the isomerization states and self-organization of this multiphotochromic compound — •Markus Koch[1,2] and Olga Guskova[1,3] — [1]Leibniz-Institute of Polymer Research Dresden, Hohe Str. 6, 01069 Dresden — [2]Institute of Theoretical Physics, Technische Universität Dresden, 01069 Dresden — [3]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden

Three-arm azobenzene derivative, a star-shaped molecule with three azobenzene (azo) groups, symmetrically attached to a central unit, has potential to be a new photooptical medium for optical recording [1]. Since it contains more than one azo-group, this system exhibits multiple isomers with diverse optical properties due to irradiation with an intensity or polarization interference pattern.

Here we show the results of DFT calculations of three-arm azo isomers, considering the changes in molecular volume, dipole moment, the first static hyperpolarizability and UV-vis spectra going from all-trans to all-cis state. Using all-atom MD simulations, we show the process of self- organization of tris(azobenzene) stars in a bulk solvent and characterize the forming clusters in terms of size, shape and stability.

We highly appreciate the financial support from DFG (project GU 1510/3-1).

[1] N.S. Yadavalli, M. Saphiannikova, S. Santer, Appl. Phys. Lett. 105, 051601 (2014).

CPP 27.3 Tue 14:30 ZEU 114

Azobenzene-containing surfactants and their association with poly(methacrylic acid) at nanometer scale — •Maria Montagna[1], Markus Koch[1,2], and Olga Guskova[1,3] — [1]Leibniz-Institute of Polymer Research Dresden, Hohe Str. 6, 01069 Dresden — [2]Institute of Theoretical Physics, Technische Universität Dresden, 01069 Dresden — [3]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden

Light-responsive hybrid materials have been considered in several recent investigations due to their promising applications in different fields, e.g. Biomedicine and Nanotechnology. One of them is azobenzene (azo), an organic chromophore which shows a reversible isomerization process between its trans- and cis-states driven by light excitation. Furthermore, the addition of this photosensitive molecule to synthetic or biological polyelectrolytes allows for remote control of the chain conformation and consequently causes changes of the polymer functional properties. We present a study on the electrostatic interaction between the azobenzene-containing surfactants and poly(methacrylic acid) by means of an atomistic computational approach. More specifically, we used a density functional theory and classical molecular dynamics simulations to look into the structural, spectroscopic and association properties of azo-polymer complexes in order to rationalize recent experimental results on the manipulation of polymer brushes modified by photosensitive molecules.

The financial support from DFG (GU 1510/3-1) is highly appreciated.

CPP 27.4 Tue 14:45 ZEU 114

Near field induced structuring of photosensitive polymer films: SNOM and AFM measurements — •Joachim Jelken, Burkhard Stiller, Carsten Henkel, Svetlana Santer, and Dieter Neher — Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany

Here we report on structuring of photosensitive polymer films by near field intensity pattern. The near fields were generated at a nano-groove fabricated within a thin metal layer. It is well known that when the nano-groove is irradiated, a surface plasmon wave is generated within the nano-groove, that should propagate along the metal surface. We have found, that instead of propagating SP mode, a standing EM-wave is generated at the metal/dielectric interface as a result of constructive interference between propagating SP mode and transmitted light. We have analyzed this phenomenon using photosensitive azobenzene containing polymer film placed above the metal surface [1-3]. The polymer film deforms following the intensity distribution of light only in case of stationary distribution of the intensity or polarization pattern. We have analyzed the system theoretically and have found that the standing wave exist even in the absence of the polymer film. This was also supported by SNOM measurements [4]. [1] T. Papke, N. Sekhar Yadavalli, C. Henkel, and S. Santer, ACS Appl. Mater. Interfaces, 6 (2014) 14174. [2] König, T.; Tsukruk V. V.; Santer, S., ACS Appl. Mater. Interfaces, 5 (2013) 6009. [3] König, T.; Yadavalli, N. S.; Santer, S., Plasmonics 7, (2012) 535. [4] J. Jelken, diploma thesis 2015.

CPP 27.5 Tue 15:00 ZEU 114

Modeling inscription of surface relief gratings on azobenzene polymers — •Marina Saphiannikova[1] and Jaroslav Ilnytskyi[1,2] — [1]Leibniz-Institut für Polymerforschung, Hohe Str. 6, 01069 Dresden, Germany — [2]Institute for Condensed Matter Physics, Svientsitskii Str. 1, 79011 Lviv, Ukraine

Azobenzene polymers proved to be invaluable in the fields of photopatterning and photomechanics. The direction of deformation can be easily controlled by illumination with linearly polarized light. Recently we showed with the help of coarse-grained simulations that a complex process of anisotropic stochastic photoisomerization can be reduced to a deterministic orientation in a field of the effective potential [1]. Presently we mimick on a coarse-grained level inscription conditions for two intensity and one polarization interference patterns commonly used to grow the surface relief gratings (SRGs). The temperature of azo-polymer film under illumination is kept very close to its value in darkness. We observe how the azo-material gradually moves from highly illuminated spots under intensity interference patterns building a sinusoidal SRG. The SRG inscribed by the polarization pattern appears to be a superposition of two SRGs inscribed by two intensity patterns, whose superposition reproduces the polarization pattern. This explains why complicated surface patterns can be inscribed using multiple steps.

[1] J.M. Ilnytskyi, M. Saphiannikova, ChemPhysChem, 16, 3180, 2015.

CPP 27.6 Tue 15:15 ZEU 114

Switching Thin Films of Metal-Organic Frameworks with Visible Light — •Kai Müller and Lars Heinke — Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

Stimuli responsive molecules, also referred to as smart molecules, change their properties when exposed to external signals like light and enable the preparation of smart materials. UV light, which often destroys organic materials, is typically required for activating the desired response of photoswitchable compounds, significantly limiting the potential applications of photoswitchable smart materials. Here, we present the first metal-organic framework (MOF) which enables reversible modulation of key properties upon irradiation with visible light only. The fluorinated azobenzene side groups can be reversibly switched between the trans and cis state by green and violet light, avoiding UV light. It is demonstrated that the uptake of guest molecules by these MOF films can be significantly increased in a fully remote controlled way. Furthermore, membrane separation experiments demonstrate the switching of the molecular separation factor by illumination with light of different color. The light-induced changes of the size of the pore windows result in the switching of the selection factor.

CPP 27.7 Tue 15:30 ZEU 114

Thin Films of Photoswitchable Metal-Organic Frameworks — •Lars Heinke — Karlsruhe Institute of Technology (KIT)

Metal-organic frameworks (MOFs) are nanoporous, crystalline materials, assembled from metal notes and organic linker molecules. In addition to many potential applications of the (conventional) powder MOF material, well-defined thin films seem perfectly suited for challenging uses and as unique model systems, where certain molecular and MOF properties can be precisely measured by applying surface sensitive techniques. These thin films are prepared in a layer-by-layer fashion on a solid substrate by using liquid-phase epitaxy, referred to as the SURMOF-approach. Incorporating photochromic molecules like azobenzene in the crystalline structure enables the switching of physical and chemical MOF properties by light. The trans-to-cis switching or vice versa of the azobenzene groups by UV or visible light, respectively, can be used for various uses, such as realizing the remote-controlled release of guest molecules from a nanoporous container. Furthermore, these films can be used as membranes for the separation of molecular mixtures. There, the photoswitchable MOF films enable a dynamic control of the selectivity by remote signals, thus enabling a continuous adjustment of the permeate flux. For H2:CO2, the separation factor can be tuned between 3 and 8 by switching the photochromic moieties. Moreover, by loading the MOF pores with conducting organic molecules, the conduction of the guest molecules can be controlled in the fully remote by trans-cis photoswitching of the host structure.

CPP 28: Focus: Soft Particles in Flows III (joint focus session CPP/DY)

Organized by S. Gekle, G. Gompper, C. Wagner

Time: Tuesday 14:00–15:45 Location: ZEU 160

Invited Talk CPP 28.1 Tue 14:00 ZEU 160

Particle based simulations of viscoelastic Soft Matter — •Wim Briels — University of Twente, Enschede, The Netherlands

In order to describe flow of soft matter in complex geometries detailed information is needed about how stresses depend on velocity gradients and concentration. Besides this, often compressible flow equations must be solved concomitantly with diffusion equations.

Since it is difficult to collect the appropriate information and to accurately represent it with a constitutive model, it is natural to develop particle based methods that can be applied to large portions of matter. In order to achieve this goal, large mesoscale objects must be represented by single particles, which move such that both the thermodynamic and the viscoelastic properties of the system are recovered.

The rheological response of Soft Matter usually results from a strong interplay between processes at all time and length scales, including the ones that have been removed by coarse graining. I will discuss a model in which the internal dynamics of the particles is reinstated through the introduction of a few structural parameters. I will apply our approach to describe the rheology of pressure sensitive adhesives and telechelic polymers. If time permits I will address some issues concerning the application of Brownian dynamics simulations of flowing soft matter in complex geometries.

CPP 28.2 Tue 14:30 ZEU 160

Telechelic star polymers under shear. — •Diego Jaramillo-Cano[1], Manuel Camargo[2], and Christos N. Likos[1] — [1]Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria. — [2]CICBA, Universidad Antonio Nariño Campus Farallones, Km 18 via Cali-Jamundí, 760030 Santiago de Cali, Colombia.

Telechelic star polymers(TPSs) are macromolecules formed by a number of diblock copolymers(arms) anchored to a common central core, being the internal monomers solvophilic and the end monomers solvophobic. Recent studies have demonstrated that TPSs constitute self-assembling building blocks with specific softness, functionalisation, shape and flexibility: depending on different physical and chemical parameters, e.g. number of arms f, solvophobic-to-solvophilic ratio α and solvent quality λ, the conformation of TSPs features a well defined number of attractive spots on the surface(patches). In this work, we exhaustively study the conformation of isolated TSPs under shear by means of a combination of MPCD for the solvent and standard MD for the monomers. By employing the Lees-Edwards boundary condition, we systematically evaluate star shape descriptors, patches distinctive features and star rotation frequency as a function of the Weissenberg number Wi for low functionality of the TPSs. We cover a wide range of parameters for representative systems given by f=18, α=0.3,0.5,0.7, λ=1.0,1.1 and Wi=1-1400. Since the conformation of single stars is expected to be preserved in low-density bulk phases, the presented results are a first step in understanding and predicting the rheological properties of semi-dilute suspensions of this kind of polymers.

CPP 28.3 Tue 14:45 ZEU 160

Soft colloid suspensions in external flow fields — •Roland G. Winkler and Gerhard Gompper — ICS and IAS, Forschungszentrum Jülich, 52428 Jülich, Germany

Soft colloids, like linear polymers as well as more complex polymeric structures such as star polymers or polymer networks exhibit large conformational changes and an intriguing dynamics when exposed to, e.g., a shear flow [1]. The flow field leads to polymer stretching, associated with a shape change of the soft colloids, and alignment, which depend on the specific structure of the particle. The particular structure even more determines the nonequilibrium dynamics. We will present simulation results of the nonequilibrium properties of such polymeric structures obtained by combining the multiparticle collision dynamics method, a mesoscale simulation approach for fluids [2], with molecular dynamics simulations for embedded polymeric objects. Moreover, the rheological characteristics of semidilute suspensions of linear [3] and star polymers [4] as well as end-functionalized semiflexible polymers [5] will be discussed.

[1] R.G. Winkler *et al.*, Curr. Opin. Colloid Interface Sci. **19**, 594 (2014)
[2] G. Gompper *et al.*, Adv. Polym. Sci. **221**, 1 (2009)
[3] C.-C. Huang *et al.*, Macromolecules **43**, 10107 (2010)
[4] S. P. Singh *et al.*, J. Chem. Phys. **141**, 084901 (2014)
[5] J. S. Myung *et al.*, J. Chem. Phys. **143**, 243117 (2015)

CPP 28.4 Tue 15:00 ZEU 160

Soft particles at a fluid interface — •Jens Harting[1,2,3], Hadi Mehrabian[2,3], and Jacco Snoeijer[3,2] — [1]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Forschungszentrum Jülich, Fürther Str. 248, 90429 Nürnberg, Germany — [2]Department of Applied Physics, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands — [3]Physics of Fluids Group, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands.

Particles added to a fluid interface can be used as a surface stabilizer in the food, oil and cosmetic industries. As an alternative to rigid particles, it is promising to consider highly deformable particles that can adapt their conformation at the interface. In this study we compute the shapes of soft elastic particles using molecular dynamics simulations of a cross-linked polymer gel, complemented by continuum calculations based on linear elasticity. It is shown that the particle shape is not only affected by the Young's modulus of the particle, but also strongly depends on whether the gel is partially or completely wetting the fluid interface. We find that the molecular simulations for the partially wetting case are very accurately described by the continuum theory. By contrast, when the gel is completely wetting the fluid interface the linear theory breaks down and we reveal that molecular details have a strong influence on the equilibrium shape. See: Soft Matter 12, 1062-1073 (2016)

CPP 28.5 Tue 15:15 ZEU 160

Migration-transition of sedimenting soft particles in vertical flows — •Andre Förtsch, Matthias Laumann, Diego Kienle, and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth

The dynamics of soft, heavy (light) particles is investigated in plane Poiseuille flows between two vertical walls and in the limit of a vanishing Reynolds number. We observe, that heavy (light) soft particles migrate to (away from) the center of a parabolic Poiseuille flow profile with the flow direction parallel to the gravitational force, similar as for buoyant particles. If the flow direction is reversed and antiparallel to gravitation, we find a surprising reversal of the migration direction and heavier (lighter) particles migrate away from (to) the center of a parabolic flow profile. This transition of the migration direction is determined numerically by the Stokesian particle dynamics and the Lattice-Boltzmann-Method as well as analytically in case of small deformations of a ring polymer. The migration away from the center is slowed down due to hydrodynamic particle-wall interactions. The parameter dependence of the final off center particle position may be used for separating different particles.

CPP 28.6 Tue 15:30 ZEU 160

Synthesis and characterization of asymmetric, viscoelastic micro-swimmers with a propulsion mechanism based on chemical reactions — •Monika Pella and Heinz Rehage — Physikalische Chemie II, Technische Universität Dortmund, D-44227 Dortmund, Deutschland

Analyzing the movement and self-organization of living cells, it is generally difficult to distinguish between physical interactions and biological processes. More detailed insights into the basic mechanisms of the swimming motions of living cells can by enabled by the investigation of artificial model swimmers. Hydrogel capsules are especially suitable for this purpose because they have similar mechanical properties as biological cells. Active chemical compounds can be stored as fuel in the core of these capsules, serving as an energy source for the propulsion of these particles. Accordingly, each swimmer has its own impellent and can move independently from each other. We investigated in different types of capsule swimmers using oxygen formation as backstroke that pushed the particles forward. Particularly the trajectories, the velocities, the attachments at solid walls, the physical-chemical properties and the typical swarming behavior of these artificial capsule swimmers are interesting. In addition to these experiments, we also analyzed the capsule swimming motion in the regime of small and large Reynold numbers.

CPP 29: Polymer Networks and Dynamics III: Mechanical Properties

Time: Tuesday 14:00–16:00 Location: ZEU 250

CPP 29.1 Tue 14:00 ZEU 250

Tuning the Properties of Polymer Films by Manipulating the Preparation Pathways — •Sivasurender Chandran, Rishab Handa, and Günter Reiter — Experimental Polymer Physics Group, Physikalisches Institut, Universität Freiburg, Freiburg, Germany

Polymer thin films take a central stage in various technological fronts ranging from polymer electronics to responsive biological surfaces. As a consequence, the ability to tune the properties of polymer films is of crucial importance. Here, through controlled manipulation of preparation pathways, we show that the final properties of pristine polymer films viz., the amount of residual stresses, elastic modulus and work for deformation, quantifying the film stability, can be tuned by orders of magnitude. Further, by identifying a normalized preparation parameter characterizing the non-equilibrium nature of polymer thin films, we deduced simple scaling relations between relaxation time and film stability with the amount of preparation induced residual stresses. Our experiments provide simple strategies for manipulating the lifetime of non-equilibrium states and hence for tuning the properties of polymer films.

CPP 29.2 Tue 14:15 ZEU 250

Analysis of entanglement effect on deformed polymer melts in non-linear viscoelastic regime — •Hsiao-Ping Hsu and Kurt Kremer — Max Planck Institute for Polymer Research

Dynamics of polymer melts are strongly affected by the entanglement effect due to the topological constraints between chains in melts both in linear and non-linear viscoelastic regime. Starting from the fully equilibrated and highly entangled bead-spring chains in melts we deform the melts by isochoric uniaxial-elongation with fixed strain rate. The strain rate is chosen such that it is fast compared to the global relaxation but slow compared to the local relaxation on the scale of the tube diameter. We study the dynamic and static properties, and the topological structures of strongly deformed polymer melts during the relaxation process in detail by molecular dynamics simulations using the package ESPResSo++. Through the primitive path analysis (PPA), the entanglement points are identified according to the curvature along the primitive path of chains. We show that the distribution of entanglement points of polymer melts becomes inhomogeneous, and the tension forces along the original and primitive paths in the stretching direction are equivalent.

CPP 29.3 Tue 14:30 ZEU 250

What controls the structure, and the linear and non-linear rheological properties of dense, dynamic supramolecular polymer networks? — •Klaus Schröter[1], Tingzi Yan[1], Florian Herbst[2], Wolfgang H. Binder[2], and Thomas Thurn-Albrecht[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg — [2]Institut für Chemie, Martin-Luther-Universität Halle-Wittenberg

Telechelic polyisobutylenes with different functional groups and a series of molecular weights were investigated by means of small angle x-ray scattering and rheology. All samples form a dense, dynamic network of interconnected micelles resulting from aggregation of the functional groups and leading to viscoelastic behavior. The dynamic character of this network manifests itself in the appearance of terminal flow at long timescales. While the elastic properties are distinctly molecular weight dependent, the terminal relaxation time is controlled by the functional end groups. The yielding properties under large deformation during startup shear experiments can be understood by a model of stress activation of the dynamic bonds. Stress relaxation experiments help to separate the non-linear response into two contributions: a fast collapse of the network and a slow relaxation, happening on the time scale of the terminal relaxation. The latter is also shown to control self-healing of the collapsed structure.

CPP 29.4 Tue 14:45 ZEU 250

Re-association dynamics of supramolecular transient networks — •Barbara Gold, Wim Pyckhout-Hintzen, Jürgen Allgaier, Andreas Wischnewski, and Dieter Richter — JCNS-1, Forschungszentrum Jülich GmbH, Wilhelm-Johnen-Straße, 52428 Jülich

Supramolecular polymers form an emerging class of smart materials bearing novel motifs such as shape memory or self-healing. Those are introduced by re-associating groups. However, a fundamental understanding of the underlying physical processes is still missing, inhibiting the design of tailor-made applications.

We present a multiple methods investigation of the dynamics of entangled supramolecular polyisoprene networks with the objective, to decipher the so far unexplained gross discrepancy between transient bond life times and rheological relaxation due to the supramolecular stickers. Information on the association constant of the functional H-bonding groups is revealed by FTIR spectroscopy while SANS measurements show a homogenous supramolecular melt. In the common temperature range the H-bond lifetime (dielectric α*-process) and the rheological relaxation differ by two orders of magnitude in time.

Within the concept of a compact random walk, where the random walker (opened sticker) undergoes multiple returns to its starting point, we quantitatively understand this so far unexplained discrepancy: The bond dissociation gives rise to the dielectric response. However, for mechanical relaxation, the association with a new partner, taking place only after multiple returns to the original binding partner, is relevant.

CPP 29.5 Tue 15:00 ZEU 250

Friction between ring polymer brushes — •Jaroslaw Paturej[1,2] and Aykut Erbas[3] — [1]Leibniz Institute of Polymer Research Dresden, 01069 Dresden, Germany — [2]Institute of Physics, University of Szczecin, 70451 Szczecin, Poland — [3]Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60208, USA

Friction between ring polymer brush bilayers sliding past each other at melt densities is studied using extensive coarse-grained molecular dynamics simulations and scaling arguments, and the results are compared to the friction between bilayers of linear polymer brushes. We show that for a velocity range spanning over three decades, the frictional forces measured for ring polymer brushes are smaller in comparison to the corresponding friction in the case of linear brushes. In the linear-force regime, the weak inter-digitation between ring brush layers as compared to linear brushes leads also to a lower number of binary collisions between the monomers from opposing brushes. At high velocities, where the thickness of the inter-digitation between bilayers is on the order of monomer size regardless of brush topology, stretched segments of ring polymers adopt the double-stranded conformation.

CPP 29.6 Tue 15:15 ZEU 250

Loss of entanglement or shear-induced ordering in polymer melts — •Ulrich Scheler — Leibniz-Institut für Polymerforschung Dresden e.V.

The transverse NMR relaxation T2 is most suited to investigate polymer chain dynamics.In polymers commonly at least two components are observed, which are attributed to the entangled and free polymer chain segments respectively. In the present study different polysiloxane melts with a narrow molecular-weight distribution have been used. Under shear in a Couette cell one commonly assumes shear-induced ordering, which would result in restricted degrees of freedom and hence a shortened T2. However in most cases a prolonged T 2 has been observed under shear, which can be explained by either a loss of entanglements or an increased mesh size between entanglements based on a local crowding of entanglements. A shortened T2 as signature of shear-induced ordering is observed only for short-chain polymers, which exhibit a single exponential decay, indicative of the absence of entanglements. That implies that the loss of entanglements is the process dominating the local polymer dynamics, while shear-induced ordering happens as well for entangled polymers.

CPP 29.7 Tue 15:30 ZEU 250

Mechanical response of soft materials at the nanoscale and the moving-surface model — •Per-Anders Thoren, Riccardo Borgani, Daniel Forchheimer, and David B. Haviland — Nanostructure Physics, KTH Royal Institute of Technology, Stockholm, Sweden

The Atomic Force Microscope (AFM) is ideal for characterization of surfaces and interfaces at the nano-scale. Despite many different measuring techniques, understanding the interaction between the AFM tip and the surface of soft materials is challenging. In most cases a Hertzian contact-mechanics model is used, where only the elastic deformation of an indented surface is considered. This approach might be justified for stiff samples, but not for soft viscoelastic materials. We present a dynamic model of both the cantilever and the soft viscoelastic surface[1]. The strong adhesion force and finite relaxation of the surface gives rise to distinct features in the oscillation amplitude dependence of the cantilevers dynamic force quadratures[2]. These dynamic force curves are easily obtained from multi-frequency AFM measurements without assuming a particular interaction model, and they separately reveal the conservative and dissipative character of the tip-surface interaction. Numerical simulation of our nonlinear moving-surface model compares extremely well to the measured force quadratures, allowing us to extract the relaxation time of the viscoelastic surface.

[1] D.B. Haviland *et al.* Soft Matter, 12, 619 (2016).
[2] D. Platz *et al.* Beilstein J. Nanotechnol. 4, 45-56 (2013).

CPP 29.8 Tue 15:45 ZEU 250

Determination of biases in equilibrium free-energy estimations from single-molecule unbinding experiments — Thomas Utzig[1], Philipp Stock[1,2], Laila Moreno Ostertag[1], and •Markus Valtiner[1,2] — [1]Max-Planck-Institut fuer Eisenforschung GmbH, Duesseldorf, Germany — [2]TU Bergakademie Freiberg, Freiberg, Germany

The capabilities of Atomic Force Microscopes to probe bond rupture at a molecular level are widely appreciated. These measurements are carried out unidirectional under non-equilibrium conditions. Jarzynski's equality (JE) has proven useful to relate the work obtained along these events to the underlying free energy of the unfolding or unbinding process. It has been also pointed out that the free energies can be biased due to finite sampling of work trajectories and dominance of rare events. Here, we present an experimental approach to quantify and correct errors arising from application of JE to single-molecule unbinding at interfaces. In particular we probe the amine/gold bond as a function of the linker's length which is used to immobilize the amine on a flat surface. With increasing linker length we observe an increase in the average work spent on unfolding and bond rupture. Also interaction energies calculated using JE increase if longer linkers are used. Our data demonstrate that the energy stored within the stretched molecule influences single molecule experiments. Further we show how these influences can be quantified, providing important design aspects for single-molecule AFM experiments.

CPP 30: Transport: Molecular Electronics and Photonics (jointly with CPP, HL, MA, O)

Time: Wednesday 9:30–12:45 Location: HSZ 201

CPP 30.1 Wed 9:30 HSZ 201

Negative differential conductance in single-molecule junctions with ferromagnetic electrodes — •Peter Hasch, Yuxiang Gong, Li Jiang, Carlos-Andres Palma, Joachim Reichert, and Johannes V. Barth — Physics Department E20, Technische Universität München, Germany

Scaling down logic operations to the level of single molecules might be considered the next frontier in computation. One approach is to electrically control single spin states in a molecule, trapped between two electrodes.

Here we report the observance of a negative differential conductance (NDC), measured in a single-molecule junction. The investigated NDC could be explained by a single-spin phenomenon, arising when the molecule gets charged due to voltage-induced depopulation of the highest occupied molecular orbital. This oxidation is monitored by Raman spectroscopy, which allows to analyze chemical and electronical structures with a single-molecule sensitivity. By (anti)ferromagnetic coupling of the unpaired spin on the molecule to one of the electrodes, the molecule might act as a spin-valve, blocking charge transport of the opposite spin direction.

Single-molecule NDC elements bear considerable potential for logical crossbar architectures, and could shrink the actual state of the art devices significantly in size.

CPP 30.2 Wed 9:45 HSZ 201

Single-molecule junctions with oligoynes and epitaxial graphene nanoelectrodes — •Konrad Ullmann[1], Susanne Leitherer[2], Maximilian Krempe[3], Rik Tykwinski[3], Michael Thoss[2], and Heiko Weber[1] — [1]Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [3]Organische Chemie I, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Single molecule junctions using graphene as electrode material have drawn considerable attention in recent years [1,2]. Due to their open access architecture, their transparency and robustness, they are well suited for a variety of unprecedented experiments. The electrode material graphene also allows for new anchor groups which connect the molecule to the electrode, e.g. via Pi-interaction.

We report on experiments using an oligoyne molecular wire with platinum termination, being contacted with epitaxial graphene nanoelectrodes. I-V characteristics show a linear behavior with a conductance close to the conductance quantum. Furthermore we present an experimental setup which uses electrospray ionisation to bring the molecules in contact with the graphene electrodes.

[1] K. Ullmann et al., Nano Lett. 15, 3512, 2015
[2] F. Prins et al., Nano Lett. 11, 4607, 2011

CPP 30.3 Wed 10:00 HSZ 201

Visualizing the role of molecular orbitals in charge transport through individual diarylethene Isomers — •Gaël Reecht[1], Christian Lotze[1], Dmytro Sysoiev[2], Thomas Huhn[2], and Katharina J. Franke[1] — [1]Freie Universität Berlin , Berlin ,Germany — [2]Universität Konstanz, Konstanz, Germany.

Diarylethene molecules are prototype molecular switches with their two isomeric forms exhibiting strikingly different conductance, while maintaining similar length. With a scanning tunneling microscope (STM) we investigate the electronic structure and the transport properties of the open and closed isomers of a sulfur-free diarylethene. The electronic structure is determined with scanning tunneling spectroscopy (STS) for the molecule lying on the surface. Between the two isomers, intriguing differences of the energy and the spatial extend of the molecule orbitals are observed. We then lift the two isomers with the tip of the STM and measure the current passing through the individual molecules. We observe an important difference of conductance between the two forms. With a simple analytical model of transport based on the results of the STS measurements, we show that the previously determined orbital characteristics are essential ingredients for the complete understanding of the transport properties.

CPP 30.4 Wed 10:15 HSZ 201

Electronic transport properties of a tripodal molecular platform — •safa golrokh bahoosh, amin karimi, elke scheer, and fabian pauly — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Intensive studies on single-molecule junctions have been performed to explore the implementation of molecular-scale devices and to understand how the molecules transport charges[1]. While molecules with delocalized π-systems are the ideal compounds to form wires for electronic applications due to their expected high conductance, tripodal molecular platforms that points almost perpendicular to the surface, appear as promising candidates to establish a conducting path between two electrodes. To take into account these aspects, a 9,9'-spirobifluorene (SBF) platform has been introduced. By combining experimental and theoretical investigations of elastic and inelastic charge transport, we show that the current proceeds through the molecular

"backbone" and identify a binding geometry that is compatible with the experimental observations in mechanically controlled break junctions[2]. The conductive molecular wire on the platform features a well-defined and relatively high conductance despite the length of the current path of more than 1.7 nm. If time permits, the possibility to use these molecules as a molecular toggle switch, as observed in subsequent studies with a scanning tunneling microscope, will be discussed.
[1] S. Aradhy, and L. Venkataraman, Nature Nanotechnol. 8, 399 (2013)
[2] M. A. Karimi, S. G. Bahoosh, M. Valášek, M. Bürkle, M. Mayor, F. Pauly, and E. Scheer, Nanoscale 8, 10582 (2016)

CPP 30.5 Wed 10:30 HSZ 201

Analysis of local current through molecular wires in open quantum systems — •Daijiro Nozaki, Andreas Lücke, and Wolf Gero Schmidt — Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany

The understanding of the local electronic flows in single molecules is of fundamental importance in the design of functional molecules as well as molecule-based electronic devices [1-4]. The charge transport through molecular wires connected between contacts is investigated using non equilibrium Green's function formalism combined with Landauer formula. Energy-dependent and total current through a series of molecular junctions are calculated in real space representation. The influence of contact positions, functional groups, and the replacement of atoms as defects on the transport properties are examined systematically. The static current-induced local magnetic field is also investigated in carbon-based molecular wires. It is shown that even in the same bias directions the direction of the magnetic field is easily reversed depending on the molecular topologies and the positions of electric contacts.
[1] M. Walz, J. Wilhelm, and F. Evers Phys. Rev. Lett. **113**, 136602 (2014)
[2] J. Wilhelm, M. Walz, and F. Evers Phys. Rev. B **92**, 014405 (2015)
[3] G. C. Solomon, C. Herrmann, T. Hansen, V. Mujica, and M. A. Ratner Nat. Chem. **2**, 223 (2010)
[4] T. Ono and K. Hirose, Phys. Rev. Lett. **98**, 026804 (2007)

CPP 30.6 Wed 10:45 HSZ 201

Controlling the conductance of graphene-molecule junctions by proton transfer — •Dominik Weckbecker, Pedro B. Coto, and Michael Thoss — FAU Erlangen-Nürnberg, Institut für Theoretische Physik, Staudtstrasse 7/B2, 91058 Erlangen, Germany

The possibility of using single-molecule junctions as components of nanoelectronic devices has motivated intensive experimental and theoretical research on the underlying transport mechanism in these systems [1]. In this contribution, we investigate from a theoretical perspective intramolecular proton transfer reactions as a mechanism for controlling the conductance state of graphene-based molecular junctions. Employing a methodology that combines first-principles electronic structure calculations with nonequilibrium Green's function transport theory [1], we show that the proton transfer reaction proceeds via a two-step mechanism and gives rise to several states of the junction with different conductance properties. In addition, we demonstrate that the relative stability of the different conductance states and the energy barriers for the interconversion reactions can be controlled by means of an external electrostatic field. The possibility of using this mechanism for the design of nanomolecular devices such as diodes or switches is also discussed [2,3].
[1] Cuevas, J. C. and Scheer, E., Molecular Electronics, World Scientific Pub. Co., Singapore, 2010
[2] Hofmeister, C. *et al.*, J. Mol. Model. **20**, 2163 (2014)
[3] Hofmeister, C. *et al.*, arXiv: 1611.01027v1 (2016)

15 min. break.

CPP 30.7 Wed 11:15 HSZ 201

Hierarchical Quantum Master Equation Approach to Vibrationally Coupled Nonequilibrium Charge Transport in Single-Molecule Junctions — •Christian Schinabeck[1], André Erpenbeck[1], Rainer Härtle[2], and Michael Thoss[1] — [1]Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany. — [2]Institut für Theoretische Physik, Georg-August-Universität Göttingen, 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 perturbative master equations. We demonstrate the importance of vibrational nonequilibrium effects for a model molecular junction consisting of an electronic level coupled to fermionic leads as well as a vibrational mode. In particular, in the off-resonant transport regime, the inelastic cotunneling signal is analyzed for a vibrational mode in full nonequilibrium, revealing a complex interplay of different transport processes and deviations from the commonly used $G_0/2$ rule of thumb [3]. Moreover, an extension of the HQME approach is presented, which allows the calculation of the full counting statistics. Using this method, the influence of higher-order cotunneling processes on the current fluctuations is analyzed.
[1] Y. Tanimura *et al.*, J. Phys. Soc. Jpn. **75**, 082001 (2006).
[2] J. Jin *et al.*, J. Chem. Phys. **128**, 234703 (2008).
[3] C. Schinabeck *et al.*, Phys. Rev. B **94**, 201407 (2016).

CPP 30.8 Wed 11:30 HSZ 201

Theoretical study of current-induced bond rupture in molecular junctions — •André Erpenbeck, Christian Schinabeck, Lukas Götzendörfer, and Michael Thoss — Institut für Theoretische Physik und Interdisziplinäres Zentrum für Molekulare Materialien (ICMM), Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany

Electronic-vibrational coupling in charge transport through single molecule junctions may result in current-induced bond rupture and is thus an important mechanism for the stability of the junction. In this contribution, we demonstrate how the hierarchical quantum master equation (HQME) theory in combination with the quasi-classical Ehrenfest approach for the nuclear degrees of freedom can be used to simulate current-induced bond rupture in single molecule junctions. Employing generic models for molecular junctions with dissociative nuclear potentials, we analyze the underlying mechanisms. In particular, we investigate the dependence of the current, the population and the dissociation probability on the model parameters. In addition, we validate the quasi-classical Ehrenfest approach using numerically exact results obtained by the HQME method [1] for a model comprising one harmonic vibrational mode.
[1] C. Schinabeck, A. Erpenbeck, R. Härtle, M. Thoss, Phys. Rev. B 94, 201407(R) (2016)

CPP 30.9 Wed 11:45 HSZ 201

Spin Transport in Helical Systems — •Matthias Geyer[1,2], Rafael Gutiérrez[1], Stefan Siegmund[3], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science, TU Dresden, 01062 Dresden, Germany — [2]Dresden Center for Computational Materials Science, TU Dresden, 01062 Dresden, Germany — [3]Center for Dynamics, TU Dresden, 01062 Dresden, Germany

Various experiments have shown strong spin selectivity in chiral molecules like DNA at room temperature. Since atomic spin orbit coupling alone is insufficient to explain the effect's magnitude, a relation to the helical geometry has been suggested. We want to provide a better understand of the underlying mechanisms by analytically and numerically investigating suitable models for electrons in helical systems with spin orbit coupling.

We follow two complementary approaches: a generic and simplified model to study the bare influence of the helical geometry and a more realistic one to calculate the effect for specific molecules. The former starts with a 3D continuum model with helix-shaped confinment from which an effective 1D Hamiltonian is derived using adiabatic perturbation theory. For the ladder an effective tight-binding model is derived from the microscopic Hamiltonian of a specific molecule. Incoherent transport calculations are performed for both models using master equations with dephasing, accounting for decoherence due to the coupling to vibrational degrees of freedom arising from structural fluctuation.

CPP 30.10 Wed 12:00 HSZ 201

Charge Carrier Dynamics in κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl: From Mott Insulator to Quantum Spin Liquid — •Jana-Isabelle Polzin[1], Benedikt Hartmann[1], Takahiko Sasaki[2], and Jens Müller[1] — [1]Institute of Physics, Goethe University Frankfurt, Germany — [2]Institute for Materials Research, Tohoku University, Sendai, Japan

The organic charge transfer salts κ-(ET)$_2$X are model systems for studying strongly-correlated charge carriers and the Mott metal-insulator transition in reduced dimensions. Recently, the influence of quenched disorder attracted considerable attention. Conducting layers of ET molecules are separated by thin, insulating sheets with anions X, resulting in a quasi-2D electronic band structure. Within the ET layers the molecules are arranged in dimers forming a triangular lattice. One free charge carrier exists per dimer, its spin being geometrically frustrated. The Mott insulator κ-(ET)$_2$Cu[N(CN)$_2$]Cl shows antiferromagnetic ordering at $T_N \approx 27\,K$. It has been shown that increasing disorder induced by X-ray irradiation drives the Mott insulating state with long-ranged antiferromagnetic order into a quantum spin liquid state [1]. Here, we discuss comparative measurements of fluctuation spectroscopy on pristine and irradiated samples in order to investigate the changes in electronic transport mechanism and low-frequency charge carrier dynamics [2] when tuning the Mott insulator to the spin liquid ground state. This results in a decrease of both resistivity and the current or voltage fluctuations after irradiation.

[1] PRL 115, 077001 (2015)

[2] PRL 114, 216403 (2015)

CPP 30.11 Wed 12:15 HSZ 201

Charge Carrier Dynamics at the Mott transition in $\boldsymbol{\kappa}$-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br — •Tatjana Thomas[1], Benedikt Hartmann[1], Takahiko Sasaki[2], and Jens Müller[1] — [1]Institute of Physics, Goethe University Frankfurt, Germany — [2]Institute for Materials Research, Tohoku University, Sendai, Japan

The organic charge transfer salts κ-(ET)$_2$X are considered as model systems for studying the Mott metal-insulator transition – a key phenomenon in the physics of strongly correlated electrons – in reduced dimensions. In particular, the influence of disorder on the criticality of the Mott transition recently has been a matter of debate. Partially deuterated κ-[(H$_8$-ET)$_{0.2}$(D$_8$-ET)$_{0.8}$]$_2$Cu[N(CN)$_2$]Br, which is located in the critical region of the phase diagram, can be fine-tuned through the Mott transition by utilizing a glass-like structural ordering transition of the ET molecules' terminal ethylene groups. By applying different thermal relaxation protocols, both the ratio of W/U and a small degree of quenched disorder can be set at will, the former corresponding to changes in hydrostatic pressure of ~ 200 bar. We employ fluctuation (noise) spectroscopy as a powerful tool to study the charge carrier dynamics at low frequencies. When crossing the S-shaped Mott transition line, surprisingly we observe a step-like increase of the resistance fluctuations in the metallic region. We discuss our results in terms of critical slowing down of the order parameter fluctuations [1] and electronic phase separation, and an extended region of the phase diagram where the fluctuations are non-Gaussian.

[1] B. Hartmann et al., *Phys. Rev. Lett.* **114**, 216403 (2015).

CPP 30.12 Wed 12:30 HSZ 201

Thermal conductance of Teflon and Polyethylene: Insight from an atomistic, single-molecule level — •Marius Buerkle and Yoshihiro Asai — AIST, Tsukuba, Japan

The thermal transport properties of teflon (polytetrafluoroethylene) and its polyethylene counterparts are, while highly desirable and widely used, only superficially understood. Here, we aim therefore to provide rigorous insight from an atomistic point of view in context of single-molecule devices. We show that for vinyl polymers adsorbed on metal-surfaces the thermal transport strongly depends one the properties of the metal-molecule interface and that the reduced thermal conductance observed for teflon derivatives originates in a reduced phonon injection life time. In asymmetric molecules phonon blocking on the intra molecular interface leads to a further reduction of thermal conductance. For hetrojunctions with different electrode materials we find that thermal conductance is suppressed due to a reduced overlap of the available phonon modes in the different electrodes. A detailed atomistic picture is thereby provided by studying the transport through perfluorooctane and octane on a single-molecule level using first principles transport calculations and nonequilibrium molecular dynamic simulations.

CPP 31: Keynote Lecture II

Time: Wednesday 9:30–10:00 Location: ZEU 222

Invited Talk CPP 31.1 Wed 9:30 ZEU 222

Using classical polymer science tools to manipulate phase transformations, solid-state order and properties of semiconducting plastics – and beyond — •Natalie Stingelin — Georgia Institute of Technology

In the past decade, significant progress has been made in the field of functional plastics such as polymeric semiconductors, ion conductors and piezoelectric polymers, with many new opportunities arising in the field of bioelectronics, energy harvesting and storage, organic electronics and photonics, and beyond. Here, examples are given of how classical polymer science tools can be utilized to gain further understanding of (multi-)functional polymers and how the physical organization, from the molecular to the macroscale of such macromolecular matter can be controlled. To this end, we present a survey on the principles of structure development from the liquid phase of this materials family with focus on how to manipulate their phase transformations and solid-state order to tailor and tune the final morphology towards technological and practical applications.

CPP 32: Organic Thin Films I (joint session CPP/DS/HL, organized by DS)

Time: Wednesday 9:30–13:15 Location: CHE 91

CPP 32.1 Wed 9:30 CHE 91

Photochromic self-assembled monolayers of phosphonate diarylethene switches on polar ZnO surfaces — •Qiankun Wang[1], Giovanni Ligorio[2], Björn Kobin[3], Stefan Hecht[3], Emil J. W. List-Kratochvil[2], and Norbert Koch[1] — [1]Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin — [2]Institut für Physik, Institut für Chemie & IRIS Adlershof, Humboldt-Universität zu Berlin — [3]Department of Chemistry, Humboldt-Universität zu Berlin

Photochromic molecular switches are attractive components in multifunctional devices, such as phototransistors and optical memories. By inserting a molecular switch interlayer into these devices, they can be used to modulate the charge injection properties by forming photoswitchable charge traps or charge barriers under the stimulation by external light. Here, we investigate the interfacial chemical and switchable properties of the phosphonic-acid diarylethene (PA-DAE) switch in form of a self-assembled monolayer (SAM) on ZnO(0001) and ZnO(000-1) surfaces by photoelectron spectroscopy. The observed work function increase is attributed to the introduced surface dipole moment; the binding modes of the phosphonate linker were retrieved from the deconvolution of core level (O 1s) spectra. Upon appropriate illumination with ultraviolet and visible light, we observe a 0.7 eV energy level shift at the onset of the highest occupied molecular orbitals (HOMO) level of the switches, which might be used to reversibly switch the energy level alignment at the ZnO/PA-DAE interface in device structures.

CPP 32.2 Wed 9:45 CHE 91

Donor-acceptor mixtures of diindenoperylene (DIP) and hexafluoro-tetracyanonaphtoquinodimethane (F6TCNNQ) studied by Polarization Modulation Infrared Reflection-Absorption Spectroscopy (PMIRRAS). New insights into the signatures of charge-transfer interactions. — •Giuliano Duva, Alexander Hinderhofer, Alexander Gerlach, and Frank Schreiber — Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

Probing intermolecular interactions in donor:acceptor (D:A) binary mixtures of organic semiconductors (OSC) [1] requires high sensitivity techniques to overcome the intrinsic limitation of having a limited amount of material and typically a weak signal. A widely used technique for studying the effects of charge-transfer (CT) interactions on molecular vibrations is Fourier-transform IR spectroscopy (FTIR) [2]. However, interference from atmospheric water and the possibly low oscillator strength of some modes may severely limit the amount of reliable information that can be extracted from the final spectrum. We present a new approach for the study of mixtures of OSCs employing PMIRRAS as high-sensitivity technique to overcome the above limitations. Supported by the structural characterization of the films via X-ray scattering, we identify and discuss the spectral signatures of CT in correlation with the formation of D:A co-crystals. [1] A. Hinderhofer et al. Chem. Phys. Chem. 13 (2012). [2] D. Nanova et al. Org. Electr. 13 (2012).

CPP 32.3 Wed 10:00 CHE 91

Coherent absorption in organic thin-film layered structures — •Tony Henseleit, Tim Wagner, Markas Sudzius, Hartmut Fröb, and Karl Leo — IAPP, Dresden, Deutschland

Development of strongly absorbing materials and devices has been a long-standing research field. Many of these efforts are based on a intriguing concept of perfect coherent absorption, which (assuming, that all required conditions are set up correctly) leads to a perfect conversion of optical energy to some form of an internal energy within the optically active material.

In this study, we focus on coherent absorption in layered thin-film structures with an organic absorbing material. The structures consist of a high optical quality dielectric distributed Bragg reflector and thermally evaporated layer of small organic molecules on it. We demonstrate both experimentally and numerically, that careful control of the resonator design and optical properties of an absorbing layer, allows to reduce amount of reflected light to the minimum and, therefore, to enhance absorption efficiency of thin organic layer up to almost 100 percent.

CPP 32.4 Wed 10:15 CHE 91

Determination of the molecular orientation in thick organic emission layers — •Christian Hänisch — IAPP, TU Dresden

The orientation of the transition dipole moment of light emitting molecules in organic thin films of up to 150nm is determined via angular resolved photoluminescence spectroscopy.

CPP 32.5 Wed 10:30 CHE 91

Influence of bulk heterojunction morphology on performances of organic solar cells — •Vladislav Jovanov, Hirwa Hippolyte, Arne Müller, Nivedita Yumnam, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

The bulk heterojunction morphology of solution processed organic solar cells can be determined by using atomic force microscopy phase imaging as we have demonstrated in our previous studies. The energy dissipated in the cantilever tip interaction with the film surface depends on the material that is present at the surface. Consequently, phase contrast is observed if different materials are forming the film surface. In this study, we have investigated the influence of a bulk heterojunction morphology on the electrical properties of organic solar cells. We have chosen a blend mixture of polymer PTB7 (donor) and fullerene PC[60]BM (acceptor) deposited from DCB/DIO solution as a materials system. In the first step, we have measured the morphologies of bulk heterojunction for different concentrations of the polymer and fullerene material. The determined structure is correlated to the electrical properties of solar cells such as short circuit current, fill factor and series resistance. The results show that bulk heterojunction morphology is crucial not only for the dissociation of generated excitons, but also for the transport of the free charge carries. Finally, we discuss the optimal organization of polymer and acceptor material.

CPP 32.6 Wed 10:45 CHE 91

The growth of α-6T on different silver surfaces — •Thorsten Wagner, Ebrahim Ghanbari, Andrea Navarro-Quezada, and Peter Zeppenfeld — Johannes Kepler University, Linz, Austria

The combination of photoelectron emission microscopy (PEEM) and differential (optical) reflectance spectroscopy (DRS) is used to compare the growth of the prototype organic semiconductor α-sexithiophene (α-6T) on different silver surfaces, namely the Ag(111), the Ag(110), and the vicinal Ag(441) surface.

An unpolarized Hg lamp was used as excitation source for the photoelectrons. For all three substrates, the transient of the mean intensity obtained with PEEM follows the same trend: The first layer decreases the emission barrier for the photoelectrons and, hence, increases the electron yield. The deposition of additional molecules just decreases the electron yield, because the electron exclusively excited from the silver substrate have to pass through the molecular layers which do not further alter the emission barrier. In all three cases, at least an equivalent of two monolayers has to be deposited before nucleation of 3D crystallites is observed in PEEM.

After being reflected at the sample surface, the light of a white LED was split by a prism into its two linearly polarized components (pol-DRS). For the isotropic Ag(111) surface, the spectra obtained for s and p polarized light do not differ qualitatively. For the Ag(110) surface, the optical spectra indicate an orientation of the α-6T molecules along the [001] direction. On the Ag(441) surface, the molecules align parallel to the steps, i.e., along the $[1\bar{1}0]$ direction.

CPP 32.7 Wed 11:00 CHE 91

How molecular quadrupole moments affect the energetics in organic thin films — •Martin Schwarze[1], Christopher Gaul[2], Katrin Ortstein[1], Frank Ortmann[2], and Karl Leo[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials, TU Dresden, 01069 Dresden, Germany — [2]Institute for Materials Science and Dresden Center for Computational Materials Science, TU Dresden, 01069 Dresden, Germany

The efficiency of organic semiconductor devices crucially depends on the precise energy level alignment of different organic layers. In most organic semiconductors, the ionization energy (IE) and the electron affinity (EA) of single molecules determine the electronic levels in organic devices and, therefore, their optimization is usually based on the IE and the EA of neat materials. However, these values can change substantially with the film morphology, at interfaces or in blends of different molecules.

By photoelectron spectroscopy, we obtain the IE of neat films at different molecular orientations and of blends with varying mixing ratios for a variety of small molecule materials. The changes of the IE, as a function of molecular orientation and mixing ratio, scale directly with the magnitude of the molecular quadrupole moments, as obtained by density functional theory simulations. By adjusting the mixing ratio of two different donor molecules, namely ZnPc and F4ZnPc, such electrostatic effects can be exploited in organic solar cells to tune the open-circuit voltage [1].

[1] Schwarze et al., Science 352, 1446 (2016)

15 min. break.

CPP 32.8 Wed 11:30 CHE 91

Correlation of Structure, Morphology, and Spectroscopic Properties of Polymorphic, Textured Squaraine Thin Films — •Frank Balzer[1], Heiko Kollmann[2], Martin Silies[2], Matthias Schulz[3], Arne Lützen[3], Christoph Lienau[2], and Manuela Schiek[2] — [1]University of Southern Denmark, Sønderborg, Denmark — [2]University of Oldenburg, Germany — [3]University of Bonn, Germany

The dihydroxy anilino squaraine 2,4-bis[4-(*N*,*N*-diisobutylamino)-2,6-dihydroxyphenyl]squaraine (SQIB) crystallizes into at least two polymorphic structures: a monoclinic and an orthorhombic phase. Spincoated thin films are, depending on the annealing temperature, highly textured with two distinct morphological features, which are assigned to the two polymorphic forms. These features exhibit different absorption spectra with characteristic spectral signatures of molecular excitons with oblique transition dipole alignment and large Davydov splitting. The monoclinic form shows a blue-shifted absorption compared to the monomer band, while the absorption profile of the orthorhombic form is red-shifted. The transitions of the excitonic states for each polymorph are polarized mutually perpendicular, probed by polarization-resolved confocal spectro-microscopy. X-ray diffraction reveals a strong out-of-plane orientation. Crystalline domains are distributed with random in-plane orientation on the samples. Their local in-plane orientation is deduced from spectro-microscopy recordings as well as from polarized light microscopy.

CPP 32.9 Wed 11:45 CHE 91

Combined structural and optical real-time study on growth of a charge transfer complex — •Valentina Belova, Alexander Hinderhfer, Alexander Gerlach, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Molecular arrangement and structure formation in binary mixed thin film organic semiconductors being in a close correlation with intermolecular interaction [1] directly influence device functionality [2]. We present a real-time investigation of structure evolution during growth (by organic molecular beam deposition OMBD) of a small-molecule donor:acceptor pair (diindenoperylene DIP : N,N0-1H,1H-perfluorobutyl-cyanoperylenediimide PDIF-CN2 [Polyera ActivInk N1100]) combining X-ray scattering methods with differential reflectance spectroscopy (DRS) in the visible range. We found strong changes in the structural and optical properties upon mixing of donor and acceptor molecules that evidence the complex formation. A strong influence of substrate temperature was observed. DRS was performed during film growth in order to establish the correlation between changes in optical spectra due to the intermolecular coupling and structural/mixing behavior. The analysis is complemented with atomic force microscopy (AFM), ellipsometry, photoluminescence and UV-Vis absorption. [1] J. Dieterle et al. J. Phys. Chem. C, 2015, 119 (47) 26339; [2] A. Opitz et al. Phys. Status Solidi A 2009, 206 (12) 2683

CPP 32.10 Wed 12:00 CHE 91

Evaluation of in-operando potential distributions in OLEDs combining experimental and drift-diffusion studies — •Maybritt Kühn[1,2], Christof Pflumm[3], Wolfram Jaegermann[1,2], and Eric Mankel[1,2] — [1]Technische Universität Darmstadt, Institute of Materials Science — [2]InnovationLab GmbH, Heidelberg — [3]Merck KGaA, department OLED-Physics, Darmstadt

Nowadays organic light-emitting diodes are widely used as displays in smart phones. As these devices consist of several functional layers it is not only important to know the driving voltage of the whole device but also the potential distributions within the single layers. Therefore we present a combined experimental and drift-diffusion study to determine in operando transport properties of the single layers. Two types of OLEDs that only differ in the emission layer but obviously exhibit different potential distributions are investigated. If the emission layer consists of TH-A a shift of the onset voltage in case of layer thickness variation can be observed while using TH-B, an isomer to TH-A, the onset voltage remains unchanged. The voltage development per layer is determined from IV curves of a set of devices with varying layer thickness. Empirically the voltage development can be described with a power law. Using the drift-diffusion model the current density dependent development of the coefficient and the exponent of the power law can be well described. With the model the mobility, the carrier injection mechanism into the respective layer and the barrier height are determined. Furthermore we are able to show that an electric field at or close to the contact is necessary to describe the TH-A behaviour.

CPP 32.11 Wed 12:15 CHE 91

Direct Micropatterning of Organic Thin Films by Electron Beam Processing — •Marie Hoffmann, Elisabeth Bodenstein, Björn Meyer, Falk Winckler, Matthias Schober, and Christoph Metzner — Fraunhofer FEP, Winterbergstr. 28, 01277 Dresden

The patterning of organic layers becomes more and more important especially for applications in solar cells and organic electronics. Organic light-emitting diodes (OLEDs) offer numerous advantages compared to commercially used LCD technology for displays and lighting, e.g. no backlight is needed and the feasibility of very thin, flexible displays is given. The improvement of OLED displays regarding efficiency, lifetime and resolution is an ongoing effort. One of the major challenges is the realization of very small structure sizes. Current patterning methods like thermal evaporation through fine metal masks, printing or lift-off techniques have been demonstrated, however, deficiencies regarding the flexibility of new applications are still existing and desired structure sizes could not be achieved jet. Therefore a method for direct patterning by using electron beam technology has been investigated. Penetrating electrons heating a multilayer system locally lead to a structured evaporation of the organic material. In the current work several experiments and investigations of electron beam processing of organic layers were performed. The process window for a careful adjustment of defined material properties could be narrowed through additional simulation calculations. First results will be shown and the technology assessed to its prospective usability.

CPP 32.12 Wed 12:30 CHE 91

Structural Properties of Thin Films of Phenacenes — •Jan Hagenlocher[1], Alexander Hinderhofer[1], Kera Satoshi[2], and Frank Schreiber[1] — [1]Eberhard Karls Universität, Tübingen — [2]Institute for Molecular Science, Okazaki, Japan

We studied the structural properties of the high band gap organic semiconductors Picene, [6]Phenacene and [7]Phenacene which exhibit high conductivity. X-ray reflectivity, grazing incidence X-ray diffraction and atomic force microscopy were applied to study the influence of a small length difference between the molecules on the crystallographic structure and morphology of the resulting mixed thin film. The compounds employed are well suited since they consist of different numbers of benzene rings fused together in a zig-zag pattern and differ only in length. It was found that the crystallographic structure remains unchanged upon mixing but the wetting behaviour, the morphology and especially the films roughness changes significantly. Different explanations are discussed and further explored using real-time X-ray reflectivity and analysis of terrace coverage of individual islands. Additionally, the optical properties of the thin films were investigated with UV-Vis spectroscopy.

CPP 32.13 Wed 12:45 CHE 91

Cyano-phenyl porphyrin on Cu(111): A STM, XPS and DFT study — •Juan Carlos Moreno-López[1], Alisson Ceccatto Dos Santos[2], Michael Lepper[3], Hubertus Marbach[3], Henry P. Pinto[1], and Abner De Siervo[2] — [1]Yachay Tech University, School of Physical Sciences and Nanotechnology, 100119-Urcuquí, Ecuador — [2]Universidade Estadual de Campinas, Instituto de Fisica "Gleb Wataghin" CP 6165, CEP 13081-970, Campinas, SP, Brazil. — [3]Lehrstuhl für Physikalische Chemie 2, Universität Erlangen-Nürnberg, Germany

The study of organic molecules on surface gained increasing interest during the last years in the research community. Studies of individual organic molecules and studies of self-assembled networks with complex interactions have shown the plausible technological applications of organic molecules on diverse fields, such as: molecular machines, molecular electronics, gas storage in molecular porous networks, etc. With this background we studied cyano-functionalized porphyrins, namely 2H-tetrakis-(p-cyano)-phenylporphyrin (2HTCNPP) on Cu(111). In this work, we performed a thorough study, by means of Scanning tunneling microscopy (STM), X-ray photoelectron Spectroscopy (XPS) and Density-functional theory (DFT) calculations, in order to gain insight into the adsorption behavior of 2HTCNPP on Cu(111) and its evolution after the deposition of Pd atoms as well as its behaviour after thermal treatment.

CPP 32.14 Wed 13:00 CHE 91

Influence of radiative efficiency and dipole orientation on optimal layer thicknesses of monochrome OLEDs for maximum EQE — •Paul-Anton Will, Cornelius Fuchs, Reinhard Scholz, Simone Lenk, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, Germany

For realizing highly efficient organic light-emitting diodes (OLEDs), the light-emitting molecule has to meet several requirements. Among chemical, energetic, and optical characteristics two crucial properties are the radiative efficiency η_{rad} and the emissive dipole orientation described by the anisotropy factor a. While the first is already close to its maximum for commonly used emitter molecules, a lot of research is currently ongoing to understand and control the dipole orientations of organic molecules. However, the external quantum efficiency (EQE) of OLEDs depends on the optical enviroment of the emitting molecules. As known, the Purcell effect leads to an effective radiative efficiency η^*_{rad} for emitters in a cavity. In this work, we show how the radiative efficiency η_{rad} and the anisotropy factor a influence the optimal layer thickness of monochrome OLEDs to reach maximum EQE. We find that for emitters with $\eta_{\mathrm{rad}} < 100\,\%$ the product of η^*_{rad} and the outcoupling efficiency η_{out} needs to be optimized, instead of solely optimizing η_{out}. When doing so, the EQE of planar OLEDs with highly oriented molecules but imperfect radiative efficiency can be pushed further. In this way, the full potential of planar OLEDs can be exploited.

CPP 33: Organic Photovoltaics and Electronics I (joint session CPP/DS/HL, organized by HL)

Time: Wednesday 9:30–12:45 Location: POT 81

CPP 33.1 Wed 9:30 POT 81

Controlling Tamm-plasmons for organic narrowband NIR photodetectors based on intermolecular charge transfer — •Andreas Mischok, Bernhard Siegmund, Dhriti Ghosh, Johannes Benduhn, Donato Spoltore, Hartmut Fröb, Christian Körner, Koen Vandewal, and Karl Leo — Dresden Integrated Center for Applied Physics and Photonic Materials, Technische Universität Dresden, Dresden

Combining a periodic distributed Bragg reflector (DBR) with a thin metal film leads to the formation of Tamm-plasmon-polaritons (TP) as sharp resonances at the DBR-metal interface. Here, we utilize such TP states to realize cavity-enhanced near infrared photodetection using an organic donor-acceptor bulk heterojunction. In such blend films, intermolecular charge transfer states play an important role during the separation of excitons. Furthermore, they can also be directly optically excited, albeit exhibiting only weak absorption coefficients and a broad linewidth. The weak extinction typically makes these states uninteresting for direct photocurrent generation, however they provide an ideal base for cavity-enhanced devices. Controlling the formation of TP resonances in a DBR-solar cell stack, we create a high-Q microcavity in the near-infrared, targeting the CT state energy. These tunable Tamm-plasmon-charge-transfer (TPCT) resonances enable direct photodetection of light well below the bandgap of the organic absorbers at zero bias and facilitate detector external quantum efficiencies of 17 % as well as a linewidth below 25 nm for spectroscopic applications.

CPP 33.2 Wed 9:45 POT 81

Field-induced exciton separation in organic solar cells: Quantifying binding energies via luminescence quenching studies — •Marina Gerhard[1], Andreas P. Arndt[2], Uli Lemmer[2,3], Ian A. Howard[3], and Martin Koch[4] — [1]Department of Chemical Physics, Lund University, 22100 Lund, Sweden — [2]Light Technology Institute, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [3]Institute of Microstructure Technology, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [4]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, 35032 Marburg, Germany

In this contribution we investigate the field- and temperature-dependence of luminescence quenching in organic solar cells (OSCs) employing a streak camera. We study the prototypical system PTB7:PC$_{71}$BM, where different emissive species i.e. singlet and CT states can be identified by choosing appropriate excitation conditions.[1] The quenching behavior and PL dynamics are satisfactorily reproduced by a kinetic model based on exciton dissociation via a hopping mechanism,[2] allowing us to take the important influence of disorder into account. Moreover, our experimental and simulative approach suggests that the binding energy of the emissive CT state (ca. 50 meV) is about one order of magnitude below that of singlet states. The absence of strongly bound CT states acting as 'deep' traps could essentially contribute to the high efficiency of the studied OSCs.

[1] M. Gerhard et al., J. Phys. Chem. C 119 (51), 2015, p. 28309

[2] O. Rubel et al., Phys. Rev. Lett. 100 (19), 2008, p. 196602

CPP 33.3 Wed 10:00 POT 81

Dissipative Charge Transfer Dynamics at an Oligothiophene/ZnO Interface — •Thomas Plehn and Volkhard May — Institute of Physics, Humboldt University Berlin, Germany

A combined theoretical study of the entire "light to free charge carrier" kinetics on hybrid organic/inorganic interfaces describes a huge challenge, owing to the manifold of interdependent subprocesses. While studies of short time quantum dynamics demand for expensive methods including e.g. electron-phonon interaction, the long time scale kinetics, however, are very sensitive to a realistic size of the model systems. In order to meet both grades, we set up an open system dynamics study based on a stochastic Schrödinger equation method.

After an introducing overview of the organic/inorganic hybrid system under consideration we present the aspired excitation energy and charge transfer processes. The presentation gives insight into the combined coherent and dissipative kinetics in a huge organic oligothiophene cluster. An initial study has the focus on solely the organic part. Then we attend to the actual hybrid interface system by placing the molecular cluster on a ZnO surface. By means of an installed electronic excess charge distribution in the inorganic counterpart, the hole motion inside the cluster becomes subject to a realistic Coulomb attraction across the interface. In order to clarify the principles of the aspired electron-hole pair separation across such interfaces, it is fundamental to understand how the hole overcomes this existing barrier.

CPP 33.4 Wed 10:15 POT 81

Charge carrier dynamics in polar organic metal-insulator-semiconductor diodes — •Alexander Hofmann[1], Simon Züfle[2], Theresa Linderl[1], Thomas Zechel[1], Lars Jäger[1], Stephane Altazin[2], Beat Ruhstaller[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]ZHAW School of Engineering, Technikumstrasse 9, 8401 Winterthur, Switzerland

Polar organic materials such as tris-(8-hydroxyquinolate) aluminum (Alq$_3$), whose strong permanent dipole moment leads to a pronounced accumulation of charge carriers at the interface, can take the role of an insulator in a metal insulator semiconductor (MIS) diode. Thus, classic wide-bandgap insulators are replaced with polar organic materials. MIS diodes in conjunction with impedance spectroscopy (IS) and charge extraction experiments (e.g. CELIV), however, represent an established device geometry to investigate charge carrier dynamics and dielectric material properties. From temperature dependent MIS-CELIV and IS on organic MIS diodes with different hole transport materials, we are able to independently determine the activation energy of hopping transport as well as the barrier for charge injection.

CPP 33.5 Wed 10:30 POT 81

Fast Organic Near-Infrared Photo-Detectors Based on Charge-Transfer Absorption — •Sascha Ullbrich, Bernhard Siegmund, Andreas Mischok, Andreas Hofacker, Donato Spoltore, Christian Körner, Karl Leo, and Koen Vandewal — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden, Dresden, Germany

In this work, we present organic near-infrared photo-detectors based on the absorption of charge-transfer states between ZnPc as donor and C$_{60}$ as acceptor material. By using a resonant optical cavity device architecture, we reach external quantum efficiencies above 1% at 1064nm for ZnPc:C$_{60}$ blends, well below (>200nm) the optical gap of the neat materials. We measure transient photo-current (TPC) responses at wavelengths of 355nm, 532nm, and 1064nm, exciting dominantly C$_{60}$, ZnPc, or the ZnPc-C$_{60}$ CT state, respectively, and obtain rise and fall times of a few nanoseconds at short circuit. We find that the response upon CT excitation is at least as fast as upon ZnPc or C$_{60}$ excitation, emphasizing the possibility to generate fast free carriers by intermolecular absorption. By reducing the active area of the devices, we are able to overcome the generally high RC time limitations caused by thin organic layers. The current transients are modeled with time dependent drift-diffusion simulations of electrons and holes which reconstruct the photo-current signal, including capacitance and series resistance effects. The hole mobility of the donor material is identified as the limiting factor for the high frequency response.

CPP 33.6 Wed 10:45 POT 81

Photovoltaic Performance of Organic Photodiodes Based on Homochiral Squaraine Compounds — •Manuela Schiek[1], Matthias Schulz[2], Majvor Mack[1], Oliver Kolloge[1], Dominik Höweling[1], and Arne Lützen[2] — [1]University of Oldenburg — [2]University of Bonn

The substitution pattern of non-toxic and environmentally stable dihydroxy-anilino squaraines [1] is modified with natural chiral functional groups such as a prolinol derivative. These natural compounds are available in their enantiomerically pure forms making costly separation of racemic product mixtures obsolete. Strong circular dichroism is measured in spin-casted thin films proving homo-chiral aggregation. Blended with a fullerene acceptor, these squaraines perform as light harvesting compound in a conventional bulk heterojunction photodiode. The performance depends on the blend ratio of squaraine and fullerene as well as on active layer thickness. In all cases, the devices suffer from low fill factors. Thinner layers lead to S-shaped current voltage characteristics around Voc. In addition, a thin active layer device with a high fullerene percentage is impacted by a photoshunt under illuminated reverse current conditions [2]. This becomes visible in reverse voltage biased EQE measurements showing a spectrally dependent deformation of the photocurrent response with the EQE exceeding 100% in the spectral response regime of the fullerene. [1] Schiek et al. Langmuir 32 (2016) 8533. [2] Tress et al. Phys. Stat. Solidi RRL 7 (2013) 401.

Coffee Break

CPP 33.7 Wed 11:30 POT 81

Hybrid solar cells from antimony sulfide nanoparticles — •wei wang, frank strössner, eugen zimmermann, kevin wong, and lukas schmidt-mende — Department of Physics; University of Konstanz

Antimony sulfide (Sb2S3) is a promising candidate for hybrid thin film solar cells due to its various favorable properties, such as suitable optical band gap (1.75 eV), high dielectric constant and good band alignment in combination with many organic hole transport materials. In our study, amorphous Sb2S3 nanospheres were fabricated by a simple colloidial synthesis method. The Sb2S3 nanoparticles were capped by oleic acid (OA) or 1-dodecanethiol (DT) molecules. Thin film hybrid solar cells were made by using these prefabricated Sb2S3 nanoparticles as absorber material by depositing them on a TiO2 covered FTO substrate. The film was then annealed to convert the particles in a crystalline film. P3HT was deposited on top as hole transporter. The device performance of the solar cells fabricated from DT capped nanoparticles was superior to the one capped with OA ligand. Fourier transform infrared spectra (FTIR) revealed that the OA molecules were still anchored to the Sb2S3 surface after high temperature annealing, while DT molecules were almost not detectable.

CPP 33.8 Wed 11:45 POT 81

Organic Light-Emitting Diodes for Optogenetic Stimulation of Neurons in *Drosophila* Larvae — •Caroline Murawski[1], Andrew Morton[1], Ifor D. W. Samuel[1], Stefan R. Pulver[2], and Malte C. Gather[1] — [1]Organic Semiconductor Centre, SUPA, School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews KY16 9SS, UK — [2]School of Psychology and Neuroscience, University of St Andrews, St Mary's Quad, South Street, St Andrews KY16 9JP, UK

Optogenetics is an emerging method in biology that enables controlling neurons non-invasively with light. Currently, however, only a small number of neurons can be controlled individually so that stimulation of neurons with light still lacks precision compared to the complexity of the brain. To overcome these limitations, we use organic light-emitting diodes (OLEDs), which enable unprecedented high-resolution optogenetic control of thousands of neurons at once. One of the challenges involves the need for very high light intensities (on the order of mW/mm^2), a brightness at which OLED efficiency typically decreases dramatically. In this contribution, we show our recent development towards achieving higher brightness OLEDs employing doped charge transport layers. Using these light sources, we demonstrate optogenetic stimulation of neurons in *Drosophila* (fruit fly) larvae and investigate subsequent behavioral changes at different light intensities.[1]

[1] A. Morton, C. Murawski, S. R. Pulver, M. C. Gather, *Sci. Rep.* 2016, **6**, 31117.

CPP 33.9 Wed 12:00 POT 81

Low Voltage Losses in Cascade Organic Solar Cells by Reducing the Donor-Acceptor Interfacial Area — •Vasileios Christos Nikolis, Johannes Benduhn, Felix Holzmüller, Christian Körner, Donato Spoltore, and Koen Vandewal — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden, Germany

High photon energy losses (E_{loss}) significantly limit the open-circuit voltage (V_{OC}) and power conversion efficiency (PCE) of organic solar cells (OSC). Reduction of E_{loss}, while keeping a high charge generation yield, can lead OSC into a new, beyond 12%, PCE regime.

In this work, we present an optimization route, which increases V_{OC} by reducing the interfacial area between electron donor (D) and acceptor (A) in planar heterojunction solar cells. Through an introduction of thin and discontinuous interlayers between D and A, we increase the V_{OC} of a cascade organic solar cell from 0.98 V to 1.16 V. Although the V_{OC} maximizes at the expense of short-circuit current and fill factor for thick interlayers, an optimum interlayer thickness for increased PCE exists. By appropriately measuring the optical gap (E_{opt}) of the device at 1.73 eV, the obtained E_{opt}-qV_{OC} losses of 0.57 eV are among the lowest observed for organic photovoltaics. Most importantly, for these devices, the external quantum efficiency (EQE) peak at the edge of the spectrum (705 nm) remains high and reaches 79%.

Our work shows that low energy losses for strongly absorbed photons can be combined with a high EQE in organic photovoltaic devices.

CPP 33.10 Wed 12:15 POT 81

Flexible organic solar cell with the effects of light trapping — •Yoonseok Park[1], Koen Vandewal[1], Karl Leo[1], Jana Ber[2,3], and Andrés Fabián Lasagni[2,3] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden, Germany — [2]Fraunhofer-Institut für Werkstoffund Strahltechnik IWS, Dresden, Germany — [3]Institute for Manufacturing Technology, Technische Universität Dresden, Germany

Organic solar cells are one of the most promising candidates for future solar power generation. They are thin and lightweight with several advantages, e. g. scalability, environmental sustainability and low cost for processing and installation. In order to set up a roll-to-roll process, flexible substrates and electrodes are required. Conventional materials, e. g. glass as substrate and ITO as electrode, are however rigid and brittle. Therefore, flexible polymer materials are investigated. Besides being flexible, polymers are much easier to process and manipulate due to their relative softness as compared to glass and metal oxides. This gives the opportunity to easily introduce light trapping structures into these materials. In this study, we apply several light trapping approaches to organic solar cells. First, PET films structured with a direct laser patterning system as well as optical display films commercially developed to be used for LCD are examined as substrates. Moreover, since PEDOT:PSS electrode is prepared by a solution-based process, nanoparticles are added as light scattering elements. Finally, 2-D nanostructures are printed by a nano-imprinting technique onto the surface of PEDOT:PSS electrodes with PDMS stamps.

CPP 33.11 Wed 12:30 POT 81

Metal-free OLEDs with organic transparent electrodes — •Irma Slowik, Axel Fischer, Paul-Anton Will, Simone Lenk, Sebastian Reineke, and Karl Leo — Technische Universität, Dresden, Deutschland

Organic light emitting devices (OLEDs) have versatile applications for flexible transparent devices as transparent displays or lightning panels. Transparent electrodes can be realized by thin metal electrodes, transparent, conducting oxides, conducting polymers, 2D materials, and metal nanowires. Organic molecular layers are mostly not suitable as electrodes due to their low conductivity, resulting in a lateral voltage drop within the organic layer and inhomogeneous emission and low efficiency of the device. However, their processing by thermal evaporation is the same as for the OLED allowing a simple fabrication process.

Here, we introduce a fully organic OLED using highly doped C_{60} as transparent electrode having a sufficiently high conductivity as well as transparency. Utilizing a tunnel junction between two highly and contrary doped semiconductors, n-doped C_{60} is suitable as top and bottom electrode, resulting in a complete organic device architecture. Although the emission decreases laterally due to the residual sheet resistance of the doped C_{60} layer, nearly uniform emission is reached within a range of several hundred microns, larger than the standard display pixel. The OLEDs provide small angular spectral shift due to the low refractive index change between electrodes and organic layers. By that approach, transparent OLEDs with bidirectional emission can be easily realized.

CPP 34: Focus: Spatio-Temporal Multiscale Optical Spectroscopy Meets Functional Materials (joint session DF/CPP/O, organized by DF)

In this Focus Session, we want to bring together scientists from transient spectroscopy as well as materials scientists, concentrating on the physics of (light-induced) excitation, transport, and relaxation in functional materials. Besides presentation of experimental techniques for spatio-temporal multiscale spectroscopy, the emphasis is laid on models and analysis tools needed to understand experimental findings beyond time constants. The Focus Session is meant to join insights and interests, potentially establishing new collaborations between "different" communities.

Organizer: Christoph Merschjann TU Berlin

Time: Wednesday 9:30–12:30 Location: GER 37

Topical Talk CPP 34.1 Wed 9:30 GER 37

Mobile electronic excitations studied by ultrafast spectroscopy — •Stefan Lochbrunner, Franziska Fennel, Steffen Wolter, and Tim Völzer — Institute of Physics, University of Rostock, Albert-Einstein-Str. 23, 18059 Rostock, Germany

The design of materials with specific photonic properties attracts currently intense scientific attention since they are the basis for many future applications in the fields of solar cells, detectors or light emitting devices. Understanding the behavior of light induced excitations in the materials is crucial for developing promising strategies. We apply time resolved spectroscopy on time scales ranging from femto- to milliseconds to characterize the sequence of processes and appearing species which result from the absorption of light. Two examples are presented in the talk. The migration of excitons due to Förster energy transfer is studied using a guest-host system based on dye molecules incorporated with a high concentration in PMMA. We characterized the influence of energetic disorder on the exciton mobility and developed a modified Förster theory which takes this effect correctly into account [1]. The dynamics of charge recombination in transition metal dichalcogenides is investigated by means of MoS_2. Evidence for defect assisted, bimolecular recombination is found by modelling the excitation dependent signal decay with corresponding rate equations.

[1] F. Fennel and S. Lochbrunner, Phys. Rev. B **92** (2015), 140301.

CPP 34.2 Wed 10:00 GER 37

Diffuse transient absorption: a tool for investigation of powdery functional materials — •Christoph Merschjann — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, D-14195 Berlin, Germany — Universität Rostock, Institut für Physik, Albert-Einstein-Straße 23-24, D-18059 Rostock, Germany

Transient absorption (TA) spectroscopy is a wide-spread and versatile tool for investigating dynamic processes induced in functional materials. Typical quantities of interest include generation, spatial transport, separation (e.g. at interfaces), and ultimate recombination of (photo)excited charge-carriers, polarons, excitons, etc.

However, most novel functional solids are initially synthesized in powder form, and many applications (e.g. catalysis) demand for rather sponge-like or otherwise rough morphologies. Standard TA spectroscopy, which typically utilizes either direct transmission or specular reflection geometries, does not perform too well for such highly scattering materials.

Here, we present a femtosecond TA spectroscopy setup using diffuse reflection/transmission geometry, showing good results for a variety of functional materials, like polymeric carbon nitrides and TaON. A major challenge is the analysis of the retrieved data. Contrary to standard TA, a simple application of Lambert-Beer's law is not possible due to a wide distribution of optical pathlengths in the sample. Models and tools for photon propagation and mutual as well as light-matter interaction, to be used alongside those models needed for the kinetics of the excited states themselves, will be discussed.

Topical Talk CPP 34.3 Wed 10:20 GER 37

Time-resolved characterization of photoactive materials using terahertz spectroscopy — •Rainer Eichberger — Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

Charge carrier mobility and lifetime are key properties of photoactive semiconductor materials. To develop and better understand novel functional materials that enable direct conversion of sunlight into electricity or chemical fuels it is essential to characterize charge generation and separation as well as carrier transport and recombination processes with high time resolution and sensitivity. In conjunction, time-resolved terahertz spectroscopy (TRTS) and microwave conductivity (TRMC) can probe a broad photoconductivity time window from a few hundred femtoseconds to milliseconds. An additional advantage of TRTS is the possibility to measure frequency-dependent conductivity or mobility spectra by transferring the signal into the Fourier space, which gives a deeper insight into the nature of carrier transport and localization. We discuss the dynamics of photo-induced processes such as polaron formation in metal oxides and charge transport issues in polycrystalline chalcopyrite and kesterite thin films arising from carrier localization caused by bandgap fluctuations.

20 min. break

Topical Talk CPP 34.4 Wed 11:10 GER 37

Theoretical simulations of pump-probe spectroscopies in solids — •Michael Sentef — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg

In this talk I will discuss recent progress of theoretical simulations of the nonequilibrium dynamics following laser excitations on femtosecond time scales. I will show two examples: (i) the nonequilibrium dynamics following laser stimulation in a cuprate high-Tc superconductor, where an electron-boson dissipation pathway could be identified in a theoretical-experimental collaboration [1,2,3]; and (ii) the proposed generation of Floquet states in solids with the prospect of engineering effective Hamiltonians [4,5]. I will use this to discuss different theoretical approaches to the nonequilibrium many-body problem - from models to materials - and the future opportunities they offer for the field of pump-probe spectroscopies.

[1] M. A. Sentef et al., Phys. Rev. X 3, 041033 (2013)
[2] A. F. Kemper et al., Phys. Rev. B 90, 075126 (2014)
[3] J. D. Rameau et al., arXiv:1505.07055 → Nature Communcations
[4] M. A. Sentef et al., Nature Communications 6, 7047 (2015)
[5] H. Hübener et al., arXiv:1604.03399 → Nature Communications

CPP 34.5 Wed 11:40 GER 37

Time-dependent quantum transport in nanosystems: A nonequilibrium Green's function approach — •Riku Tuovinen — Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, 22761 Hamburg, Germany — Department of Physics, Nanoscience Center, FIN 40014, University of Jyväskylä, Finland

Quantum transport is often discussed in the steady-state regime where the characteristics of the system are described in terms of the energy-dependent transmission or conductance. It is not guaranteed, however, that this description would capture the essential physics in, say, atomic-scale junction operating at high frequencies. Therefore, we consider the full time-dependence which also provides us with "transient spectroscopy" giving detailed information about the nanosystems out of equilibrium. A time-dependent extension to the Landauer–Büttiker approach is presented. The nonequilibrium Green's function approach is employed for describing the charge and heat transport dynamics. The importance of the method is that it provides a closed formula for the time-dependent density matrix in both electronic and phononic systems. In the electronic case the nonequilibrium conditions are due to a switch-on of a bias voltage in the leads or a perturbation in the junction whereas in the phononic case the junction is coupled to reservoirs of different temperatures. In both cases time-dependent transport properties, such as local charge and heat currents, may be evaluated without any propagation. Some applications with, e.g., graphene-based circuitries are presented and discussed.

Topical Talk CPP 34.6 Wed 12:00 GER 37

Accessing micro- and mesoscopic ultrafast electron dynamics in low-dimensional materials — Michele Puppin[1], Christopher Nicholson[1], Melanie Müller[1], Roman Bertoni[1], Hannes Hübener[2], Angel Rubio[2], Claude Monney[3], Cephise Cacho[4], Martin Wolf[1], Alexander Paarmann[1], Laurenz Rettig[1], and •Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin — [2]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg — [3]Universität Zürich, CH — [4]STFC Rutherford Appleton Laboratory, UK

The coupling of electronic, phononic and spin degrees of freedom is at the heart of most phenomena in condensed matter and governs the flow and relaxation of charge carriers in out-of-equilibrium conditions. Microscopic coupling and correlation effects can be accessed quantitatively by time-, energy- and momentum-resolved information on ultrafast electron dynamics as obtained by time- and angle-resolved photoelectron spectroscopy (trARPES). I will discuss the generation of spin-, valley- and layer-polarized excited states in the semiconductor WSe_2 [1], their ultrafast evolution from 2D to 3D states, and the signatures of transient excited-state many-body interactions. In addition, the visualization of the spatio-temporal evolution of photocurrents in a nanowire by means of femtosecond point-projection microscopy will be discussed [2,3].

[1] Bertoni *et al.*, Phys. Rev. Lett., in print, arXiv:1606.03218.
[2] Müller *et al.*, Nature Comm. 5, 5292 (2014).
[3] Müller *et al.*, ACS Photonics 3, 611 (2016).

CPP 35: Focus: Polymer Crystallization - from Model Systems to New Materials I

Organisers: Jens-Uwe Sommer (IPF Dresden), Thomas Thurn-Albrecht (Martin-Luther-Universität Halle)

Polymers with special semicrystalline morphologies play a key role in current research as e.g. in polymeric semiconductors, in the crystallization in polymer networks or in crystalline biopolymers. Notably, the physics of polymer crystallization itself is a topic of ongoing debate. This focus session aims at highlighting selected fundamental and applied aspects of polymer crystallization and at bringing together contributions from different fields to enable common discussions and exchange.

Time: Wednesday 10:15–13:00 Location: ZEU 222

CPP 35.1 Wed 10:15 ZEU 222

Characterization of polymer crystallization in conducting thin films using grazing incidence x-ray scattering — Stephan Pröller[1], Jenny Lebert[1], Mihael Coric[1], Peter Müller-Buschbaum[2], Alexander Hexemer[3], and •Eva M. Herzig[1] — [1]TU München, Munich School of Engineering, Herzig Group, 85748 Garching, Germany — [2]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [3]Lawrence Berkeley National Laboratory, Advanced Light Source, Berkeley, USA

The material properties of conducting thin films are - like for many other material systems - closely linked to the nanoscale order and disorder of the involved polymers. Therefore it is important to have adequate experimental methods allowing the characterization of crystallization and aggregation of polymers in thin films, and ideally also during thin film formation. Grazing incidence wide angle x-ray scattering is more and more frequently used to examine the nanoscale order in thin films. Using examples of model systems and novel materials studied in our group the capabilities and limitations of this method are demonstrated.

CPP 35.2 Wed 10:30 ZEU 222

Controlled Crystallization of n-type Semiconducting Polymer Thin Films — •Sabine Ludwigs — Institute of Polymer Chemistry, University of Stuttgart

This contribution will focus on current activities in my group on thin films of n-type semiconducting poly[N,N*-bis(2-octyldodecyl)-1,4,5,8-naphthalene-dicarboximide-2,6-diyl]-alt-5,5*-(2,2*-bithiophene) (PNDI2OD-T2) and its regioirregular analogues. The assignment of these donor-acceptor copolymers as conjugated redox polymers will be discussed based on electrochemical and field effect transistor measurements.(1,2) Solvent vapor annealing proves to be an excellent tool to obtain spherulitic structures with controlled nucleation density and crystalline order over large areas in thin films.(3) The role of post-annealing procedures to tailor textures and polymorphism will be further highlighted. (1) D. Trefz et al. J. Phys. Chem. C 2015, 119, 22760. (2) Y. Gross et al. Tuning aggregation by regioirregularity in n-type P(NDI2OD-T2) donor-acceptor copolymers, 2017, to be submitted. (3) G. Schulz, S. Ludwigs Adv.Funct.Mater. 2016 DOI: 10.1002/adfm.201603083.

CPP 35.3 Wed 10:45 ZEU 222

In-operando study of changes in the crystalline parts of P3HT:PCBM solar cells — Daniel Moseguí González[1], Christoph J. Schaffer[1], Stephan Pröller[2], Johannes Schlipf[1], Lin Song[1], Sigrid Bernstorff[3], Eva M. Herzig[2], and •Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]TU München, MSE, Lichtenbergstr. 4, 85748 Garching — [3]Elettra-Sincrotrone Trieste, 34149 Basovizza, Italy

Organic solar cells based on poly(3-hexylthiophen-2,5-diyl):phenyl-C60-butyric acid methyl ester (P3HT:PCBM) have developed into a well-controlled model system for studying fundamental questions, although device efficiencies of other blends using low band gap polymers demonstrated significantly higher device efficiencies. Based on an in-operando investigation of a P3HT:PCBM-based solar cell we address for the first time the correlation between the crystalline state of the materials in the organic solar cell and the open circuit voltage probed in the IV-characteristics. We use in-operando grazing incidence wide angle x-ray scattering to probe changes in the crystalline parts of the active layer. The findings give a better understanding of aging of organic solar cells during operation.

CPP 35.4 Wed 11:00 ZEU 222

Impact of Molecular Dynamics on Structure Formation of Donor-Acceptor Block Copolymers — •Matthias Fischer[1], Christian David Heinrich[2], Mukundan Thelakkat[2], and Thomas Thurn-Albrecht[1] — [1]Martin Luther University Halle-Wittenberg — [2]University of Bayreuth

Donor-Acceptor block copolymers (BCP) are attractive materials for organic photovoltaics due to their intrinsic property to form an equilibrium nanostructure on the length scale of exciton diffusion. As usually semiconducting polymers are crystalline or liquid crystalline structure formation is complex in these BCPs. We here present a study of the interplay between phase separation, crystallization and glass transition in two donor-acceptor BCPs of poly(3-hexylthiophene)-block-poly perylene bisimide (P3HT-b-PPBI) incorporating P3HT as donor and polystyrene with two different pendant perylene bisimides as acceptor. In order to study the effect of backbone glass transition on side chain crystallization in the acceptor block low molecular weight model compounds, homopolymers and BCPs were compared using differential scanning calorimetry and temperature dependent wide- and small-angle x-ray scattering as central methods. While microphase separation in the liquid state led to a cylindrical morphology in both cases the crystallization of the side chains depended strongly on the backbone glass transition temperature as compared to the ordering temperature of the PBI units. Surprisingly, a strong π-π-interaction was found even in the absence of lateral ordering of the side chains possibly explaining the relatively high electron mobility of these disordered materials.

CPP 35.5 Wed 11:15 ZEU 222

Structural in-operando investigations on PEDOT:PSS electrodes under high humidity conditions — •Lorenz Biessmann[1],

Markus Trunk[1], Bo Su[1], Hong Xu[1], Sigrid Bernstorff[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Elettra-Sincrotrone Trieste, 34149 Basovizza, Italy

Towards flexible substrates for organic light emitting diodes and organic photovoltaics it is of significant interest to get rid of brittle, costly electrodes like ITO or FTO as well. PEDOT:PSS offers with its good conductivity, easy processibility, and inherent flexibility a suitable alternative to its rigid and transparent conducting oxide counterparts. The crystallinity as well as orientation of crystals in PEDOT:PSS films is known to have a significant influence on the film conductivity. In particular, the appearance of water in air can cause oxidation and thus decrease the device efficiency or cause device failures. Therefore, we investigate changes of the crystal structure of spray-deposited PEDOT:PSS films under high humidity conditions. We monitor changes in crystallinity and orientation of crystals with in-operando grazing incidence wide angle x-ray scattering (GIWAXS). The variation of conductivity of PEDOT:PSS is linked to the GIWAXS findings. Furthermore, reversibility is studied.

15 min break

Invited Talk CPP 35.6 Wed 11:45 ZEU 222

Density functional theory of crystallization: from anisotropic particles to polymers — •Hartmut Loewen — Universitaetsstrasse 1, 40225 Duesseldorf

Classical density functional theory for freezing is used to predict the equilibrium bulk phase diagram of anisotropic particles. Explicit results are obtained for orientable hard rectangles in 2 spatial dimensions where isotropic, nematic and smectic phases do occur as a function of particle aspect ratio and number density. Then the density functional theory is applied to the smectic phase on a nontrivial curved manifold like a cone. Confinement-induced phase transition are calculated. Last, ideas to extent the theory towards polymer crystallization are described.

CPP 35.7 Wed 12:15 ZEU 222

Real-time observation of non-classical protein crystallization — •Benedikt Sohmen[1], Marcus Mikorski[1], Andrea Sauter[1], Felix Roosen-Runge[2], Ralf Schweins[2], Fajun Zhang[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany — [2]Institut Laue-Langevin, Grenoble, France

In order to approach a better understanding of non-classical crystallization a huge diversity of mechanisms has been discussed recently [1,2]. Here, we present a combined SAXS and SANS real-time study of the crystallization pathways of β-lactoglobulin in the presence of $CdCl_2$ with respect to protein concentrations c_p and salt concentrations c_s. Depending on the location in the c_p-c_s phase diagram, different crystallization pathways are observed. For $c_s < c^*$, the solutions are clear and crystallization follows a classical one-step pathway. For $c^* > c_s > c^{**}$, the system enters a condensed regime where an intermediate phase prior to crystallization is observed. By investigating the structure and the temporal evolution of the intermediate phase we clarify its role with respect to crystallization. Based on our studies, we suggest that β-lactoglobulin can follow different non-classical crystallization pathways. The intermediate phase can act as both, a material reservoir and a crystal precursor. [1] De Yoreo et al., Science, **349**, 2015, 6760 [2] Sauter et al., J. Am. Chem. Soc., **137**, 2015, 1485-1491

CPP 35.8 Wed 12:30 ZEU 222

Lattice free energy functional for anisotropic particles with pure hard–core interaction and with short–ranged attractions — •Mostafa Mortazavifar and Martin Oettel — Institut für Angewandte Physik, Eberhard Karls Universität Tübingen, Tübingen, Germany

By using a free energy functional of fundamental measure type, the equilibrium properties of a pure hard–rod mixture and hard rods with short–ranged attractions are investigated in a lattice model where the position and the orientation of rods are restricted to discrete values. Attractions are incorporated via one or more species of polymeric lattice particles in the spirit of the Asakura–Oosawa model. By changing size and shape of these particles, effective attractions of different strength and range can be generated.

We have investigated phase diagrams of 2– and 3–dimensional bulk systems and of monolayers formed with 3–dimensional rods. Bulk 3–dimensional systems exhibit liquid–vapor and isotropic–nematic transitions similar to the systems with rods in continuum. For the monolayers, the continuous nematic transition remains present above a critical temperature and is superseded by a gas–liquid transition below the critical temperature.

CPP 35.9 Wed 12:45 ZEU 222

Small polyethylene systems: On the ground state of single chains and few chain aggregates — •Timur Shakirov and Wolfgang Paul — Institute of Physics, University of Halle, Halle, Germany

The phase behavior of polyethylene has been under investigation for the last six decades. Investigation of single-chain crystallization in solution is a technically difficult problem, because in molecular dynamics simulations as well as in experiments, it is not so easy to distinguish kinetic and thermodynamic effects on chain folding. The general picture, however, is, that single polyethylene chains in solution fold into lamellar crystals. We present results of a Stochastic Approximation Monte Carlo (SAMC) simulation, which gives a possibility to analyze thermodynamical equilibrium properties of a system. Our simulation study of relatively short polyethylene chains is based on a chemically realistic united atom model [1]. Simulational results for low-energy states of single chains of different lengths demonstrate a set of various ground-state configurations: from stretched and hairpin-like configurations of short chains to a helix-like structure reeled round one of the chain*s ends. Aggregates of a few short polyethylene chains exhibit another set of ground states, depending on chain length and number of aggregated chains. However, with increasing chain length, single chain and aggregate morphologies become more similar.

[1] W. Paul, D. Y. Yoon, and G. D. Smith, J. Chem. Phys. 103 (1995) 1702-1709.

CPP 36: Colloids and Complex Fluids II (joint session BP/CPP/DY, organized by CPP)

Time: Wednesday 10:15–13:00 Location: ZEU 260

Invited Talk CPP 36.1 Wed 10:15 ZEU 260

Computer simulations of colloidal systems under flow — •Arash Nikoubashman — Institut für Physik, Johannes Gutenberg-Universität Mainz, Mainz, Germany

Colloidal systems under flow are ubiquitous in nature and technology, whether it is the transport of proteins and enzymes in biological systems or the flow of surfactants in enhanced oil recovery. Such microrheological systems are also highly intriguing from a purely scientific point of view due to the intricate interplay between the solute and solvent particles. To better understand the physical properties of these complex systems and to assist the design of microfluidic devices, we performed extensive simulations of both rigid and soft colloidal particles under flow. This computational approach allows for systematic control over the system parameters while also providing microscopic insight. In this presentation, selected systems will be discussed to give an overview of the possibilities and challenges in this field. For example, microfluidic channels can be used to distinguish polymers based on their topology, such as linear, dendritic or ring-shaped macromolecules. Furthermore, non-linear flow effects such as inertia or viscoelasticity can be exploited to control the lateral motion of dispersed particles. Flow can also be used to enhance the growth as well as the breakup of colloidal aggregates, depending on the applied flow strength.

CPP 36.2 Wed 10:45 ZEU 260

A temporarily arrested state in protein solutions — •Stefano Da Vela[1], Fajun Zhang[1], Christian Exner[1], Johannes Möller[2], Zhendong Fu[3], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]ESRF, Grenoble, France — [3]JCNS, Garching, Germany

The interplay of liquid-liquid phase separation (LLPS) with the glass transition is a possible route to the formation of arrested states in colloidal and protein systems. LLPS requires attractive interactions, the microscopic details of which set the temperature dependence of the LLPS phase boundary. We report the kinetics of phase separation and arrest for two protein systems: γ-globulin in the presence of PEG 1000, featuring upper critical solution temperature behavior, and bovine serum albumin in the presence of Y(III), featuring lower critical solution temperature behavior. For both systems, the time evolution of the characteristic length is followed during phase separation by Ultra Small Angle X-ray Scattering (USAXS) and Very Small Angle Neutron Scattering(VSANS). This time evolution corresponds to classical LLPS proceeding by spinodal decomposition for shallow quenches in the two-phase region, and to arrested LLPS for deep enough quenches [1]. For intermediate quenches, we report evidence of an unusual three-stage coarsening process. In this case, a temporary arrest of the kinetics is found, which is overcome at later times. We interpret the finding in the light of simulations and experimental results on colloidal systems.

[1] Da Vela et al. Soft Matter, 2016, 12, 9334 - 9341

CPP 36.3 Wed 11:00 ZEU 260

Demixing and clustering in a binary system of long-ranged capillary interactions — •Malte Lütje, Johannes Bleibel, and Martin Oettel — Institut für Angewandte Physik, Universität Tübingen, Deutschland

We consider a binary system of micron-sized spherical colloidal particles trapped at a fluid interface, which induces long-ranged capillary interactions. If one species has positive and one has negative buoyancy, colloids of the same species attract while different species repel. This leads to the demixing of initially uniform densities, and ultimately to the formation of close-packed clusters for each species. Demixing competes with the clustering of each species.

We present static phase diagrams for the system. Brownian Dynamics simulation results illustrate the evolution from a homogeneous state to the demixed and clustered states. The system has unusual phase separation dynamics: The timescales of demixing and clustering can be different, yielding an intermediate stage with halo-like structures.

CPP 36.4 Wed 11:15 ZEU 260

Poisson-Boltzmann study of the effective electrostatic interaction between colloids at an electrolyte interface — •Arghya Majee[1,2], Markus Bier[1,2], and S. Dietrich[1,2] — [1]Max-Planck-Institut für Intelligente Systeme, Heisenbergstr. 3, 70569, Stuttgart — [2]IV. Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70569, Stuttgart

The effective electrostatic interaction between a pair of colloids, located close to each other at an electrolyte interface, will be discussed by employing the full, nonlinear Poisson-Boltzmann (PB) theory within classical density functional theory. Using a simplified yet appropriate model, all contributions to the effective interaction are obtained exactly, albeit numerically. The comparison between our results [1] and those obtained within linearized PB theory [2] reveals that the latter overestimates these contributions significantly at short inter-particle separations. Whereas the surface contributions to the linear and the nonlinear PB results differ only quantitatively, the line contributions show qualitative differences at short separations. Moreover, a dependence of the line contribution on the solvation properties of the two adjacent fluids is found, which is absent within the linear theory. Our results are expected to enrich the understanding of effective interfacial interactions between colloids.

References:

[1] A. Majee, M. Bier, and S. Dietrich, J. Chem. Phys. **145**, 064707 (2016). [2] A. Majee, M. Bier, and S. Dietrich, J. Chem. Phys. **140**, 164906 (2014).

15 min break

CPP 36.5 Wed 11:45 ZEU 260

Entropic Interactions between Dendrimers and Impenetrable Surfaces — •Ron Dockhorn[1,2], Stephan Meschede[3], Martin Wengenmayr[1,2], and Jens-Uwe Sommer[1,2] — [1]Leibniz Institute of Polymer Research Dresden, D-01069 Dresden, Germany — [2]Technische Universität Dresden, Institute for Theoretical Physics, D-01069 Dresden, Germany — [3]Institute for Physics, Humboldt-Universität zu Berlin, D-12489 Berlin, Germany

Monte Carlo simulations are performed to investigate depletion effects on dendrimers using the bond fluctuation model. Two different situations are investigated: The interaction between a single dendrimer against a hard wall and the interaction between two dendrimers. The simulations of the dendrimers are performed with implicit solvent as well as in a linear polymer matrix. The free energy landscape along the particular reaction coordinate is determined by Umbrella Sampling (WHAM algorithm) and compared to a mean-field approach. Both systems immersed in a polymer matrix show entropic attraction (depletion forces) depending on the length of the surrounding linear chains. Additionally, a spontaneous conformational change and rapid mixing caused by the strong interaction in the two dendrimers' system can be noticed. These findings are aimed to understand the agglomeration and the coagulation processes of hyperbranched structures in drug-delivery systems in medical applications.

CPP 36.6 Wed 12:00 ZEU 260

Liquid-state theory of the interactions between colloids mediated by attractive reversibly adsorbed polymers. — •A.I. Chervanyov — Institute for Nano- and Microfluidics, TU Darmstadt

By making use of the liquid state theory, we analytically study the effect of attractive polymer-colloid (P-C) and polymer-polymer (P-P) interactions on the effective forces acting between colloids immersed in a polymer system. The performed theoretical analysis has no restrictions with respect to the polymer density and relative sizes of the colloids and polymers. The polymer mediated (PM) potential acting between fillers is shown [1,2] to significantly depend on the strength and range of the P-P and P-C interactions. In the nano-particle limit, where the colloid radius is much smaller than the polymer gyration radius, the presence of attractive P-P interactions causes significant, but only quantitative changes to the PM potential. In the opposite limit of relatively large colloids, the P-P interactions revert the sign of the total effective force acting between colloids so that this force becomes attractive at sufficiently large polymer densities. The effect of the C-P interactions on the PM potential is found to be most pronounced in the case of large polymer densities and small colloid-to-polymer size ratios. The dependence of the second virial coefficient of the effective PM potential on the polymer density is discussed in detail, revealing several novel features of the PM forces caused by the presence of attractive P-P and P-C interactions.

[1] A.I. Chervanyov, Soft Matter 11,1038-1053 (2015).

[2] A.I. Chervanyov, J. Chem. Phys. 141, 244902(2014).

CPP 36.7 Wed 12:15 ZEU 260

Determing helicity modulus in systems with orientational order from microscopic properties through Zwanzig-Mori formalism — •Johannes Häring and Matthias Fuchs — FB Physik, Universität Konstanz, 78457 Konstanz, Germany

Up to now, we have studied crystals with point disorder and applied the theory to crystals of soft core particles, so-called cluster crystals [1]. Now, systems with orientational order like nematic liquid crystals are considered. With the Zwanzig-Mori formalism it is possible to calculate the helicity modulus for all temperatures in the ordered phase, even near the critical point.

The Zwanzig-Mori formalism is a way to treat many-body systems systematically. Projection Operators are used to focus on the dominant variables of the system and their correlation functions. Simulations of the three dimensional XY model are done to test the accuracy of the approach. The XY model consists of particles with one orientational degree of freedom which are fixed on a lattice.

It is known from the Mermin-Wagner theorem that two dimensional systems show no conventional long range order, i.e have vanishing order parameters. That leads to problems in calculating the helicity modulus. We discuss how it is still possible to obtain a solution.

[1] J. M. Häring, C. Walz, G. Szamel, and M. Fuchs, Phys. Rev. B 92, 184103 (2015)

CPP 36.8 Wed 12:30 ZEU 260

Clusters in dipolar fluids — •Michela Ronti[1], Alexey O. Ivanov[2], Lorenzo Rovigatti[3], Jose M. Tavares[4], Francesco Sciortino[5], and Sofia S. Kantorovich[1,2] — [1]Computational Physics, University of Vienna, Sensengasse 8, 1090 Vienna, Austria — [2]Ural Federal University, 3 Ural Federal University, Lenin av. 51, Ekaterinburg, 620000, Russia — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, 1 Keble Road, Oxford, OX1 4 NP, United Kingdom — [4]Instituto Superior de Engenharia de Lisboa-ISEL, Rua Conselheiro Emidio Navarro 1, 1950-062 Lisboa, Portugal — [5]University of Rome La Sapienza, Piazzale Aldo Moro 2, I-00185, Roma, Italy

We describe the self-assembly in magnetic nanocolloids by using a dipolar hard sphere (DHS) model. The phase diagram of this system at low temperature remains debatable regardless the expected simplicity of the model. At low temperature DHS particles self-assemble into complex structures, with primary structures composed by rings and chains. The latter form the building blocks for further aggregation. To elucidate the formation of branched structures analytically, we need to calculate accurately partition functions of various clusters. For that we introduce grand-canonical single cluster Monte Carlo simulations.

CPP 36.9 Wed 12:45 ZEU 260

Ferromagnetic phases in colloidal suspensions — •Grigorii Zarubin[1,2] and Markus Bier[1,2] — [1]Max Planck Institute Int. Sys. — [2]University of Stuttgart, Germany

A ferromagnetic phase of anisotropic particles suspended in a nematic liquid crystal (NLC) was predicted as early as 1970 [1]. A recent experimental realization [2] confirmed that a dilute suspension of magnetic platelets in NLC forms ferromagnetic phase which is susceptible to weak magnetic fields. In this work we describe such a suspension of plate-like particles using density functional theory. The influence of the NLC is taken into account implicitly through the introduction of the effective elastic interaction between platelets. Following approach of Lev and Tomchuk [3], the effective potential was derived under the assumption of weak anchoring of the NLC at the surface of the platelets. An ordered phase was identified with help of the orientational distribution function, and the dependence of the ferromagnetic phase on the strength of the magnetic and the elastic coupling was studied.

References: [1] F. Brochard and P.G. de Gennes, J. Physique 31, 691 (1970). [2] A. Mertelj, D. Lisjak, M. Drofenik and M. Copic, Nature 504, 237 (2013). [3] B.I. Lev and P.M. Tomchuk, Phys. Rev. E 59, 1 (1998).

CPP 37: Fluids and Glasses I

Time: Wednesday 10:15–13:00 Location: ZEU 255

CPP 37.1 Wed 10:15 ZEU 255

Effects of the molecular polarity on the structural and dynamical properties of liquid silica — •Elvira Pafong and Barbara Drossel — Institut für Festkörperphysik, Technische Universität Darmstadt

Silica is a network-forming liquid that shares many properties with water. Both liquids are polar, which leads to directional bonds and complex structural and dynamical features. In particular, liquid silica undergoes a transition from a strong to a fragile glass former, comparable to the transition from a high-density liquid (HDL) to a low-density liquid (LDL) reported in water. Here, we investigate the effect of the molecular polarity on the structure and dynamics of liquid silica using molecular dynamics simulations. We modify polarity by changing the partial charges assigned to each atom. We find that the glass forming ability of liquid silica is enhanced by an increase of the partial charges of up to +20%. The temperature corresponding to the maximum or the minimum in density, the average tetrahedral order parameter as well as the correlation times increase also. Interestingly, when the partial charges are increased further to +30%, a fifth atom enters the first neighbouring shell for temperatures above 4000 K, resulting in a structure that is locally less ordered and therefore in less pronounced anomalies.

CPP 37.2 Wed 10:30 ZEU 255

Metabasin Lifetimes of Sheared Supercooled Liquids — •Markus Blank-Burian and Andreas Heuer — Institut für Physikalische Chemie, WWU Münster, Deutschland

In the limit of small shear rates and temperatures around the glass transition temperature T_g, a sheared supercooled liquid can be described by hopping processes between so called metabasins [1]. However, in the limit of small temperatures and high shear rates the dynamics can be described by vanishing energy barriers in the PEL [2].

We analysed this crossover region with molecular dynamics simulations at various temperatures ($0.01 \leq T \leq 1.0$) and shear rates ($10^{-6} \leq \dot{\gamma} \leq 10^{-1}$). A very small system size ($N = 130$) was used, which is not affected by major finite size effects. A plastic event in this system size typically spans the whole box, so that the system does not show shear banding.

We can show, that two simple models, describing the metabasin lifetimes under constant shear rate and finite temperature, are in good agreement with our numerical data. The first model assumes that the metabasin energy dependent activation barriers are continuously reduced by shearing the system. The second, more simplistic model, assumes a superposition of transition rates, reflecting the limit of low temperature and the limit of low shear rates, respectively, to characterize the transition region between temperature- and shear-dominated dynamics.

[1] A. Heuer, J. Phys.: Condens. Matter 20, 37 (2008)
[2] D. J. Lacks, Phys. Rev. E 66, 5 (2002)

CPP 37.3 Wed 10:45 ZEU 255

Dielectric Spectroscopy Below the Glass Temperature — •Korbinian Geirhos, Peter Lunkenheimer, and Alois Loidl — Experimental Physics V, University of Augsburg, Germany

The dynamics of glassy matter above the glass temperature ($T_{\rm g}$) is already extensively studied by dielectric spectroscopy in a broad frequency and temperature range. Dielectric data of glasses below $T_{\rm g}$, however, are rather scarce. The dielectric spectra of glass formers above $T_{\rm g}$ are dominated by relaxation processes. These contributions may hide additional processes, which are proposed by different models, like the "Nearly Constant Loss" of the Coupling Model [1] or the fast β-Process of the Extended Mode Coupling Theory [2]. Below $T_{\rm g}$, however, the main relaxation features are shifted out of the experimental frequency window. As a consequence, possible additional processes can be observed and studied. For this purpose, we provide temperature- and frequency-dependent dielectric data of different glass formers down to temperatures of 4 K.
[1] K. L. Ngai, J. Phys.: Condens. Matter **15**, 1107 (2003). [2] W. Götze *et al.*, Rep. Prog. Phys. **55**, 241 (1992).

CPP 37.4 Wed 11:00 ZEU 255

Dynamic glass transition in the supercooled liquid and plastic crystal of ethanol — •Yeong Zen Chua[1], Amanda R. Young-Gonzales[2], Ranko Richert[2], and Christoph Schick[1] — [1]Institut für Physik, Universität Rostock, Rostock, Germany — [2]School of Molecular Sciences, Arizona State University, Tempe, Arizona, USA

Ethanol has been widely investigated and is well-known to exhibit a very interesting polymorphism of different solid phases: a fully-ordered (monoclinic) crystal, a (bcc) plastic crystal, a glassy plastic crystal and an ordinary amorphous glass. Physical vapor deposition (PVD) has been used to prepare amorphous glasses of ethanol, which upon heating to higher temperature transforms into the plastic crystal of ethanol. The dynamic glass transition of supercooled liquid of ethanol is successfully measured by AC nanocalorimetry. Preliminary results for the plastic crystal are also presented. With that, the frequency dependency of the dynamic glass transition of the supercooled liquid of ethanol is measured and compared with published dielectric data. Comparison of dielectric data of supercooled liquid of ethanol with AC nanocalorimetric data shows that ethanol exhibits Debye peak, which cannot be observed in AC nanocalorimetry. In previous published dielectric data, the prominent Debye peaks have been mistaken as structural α relaxation. The dielectric data have been re-evaluated and the high frequency wing in the dielectric spectra is identified as the structural α relaxation.

Invited Talk CPP 37.5 Wed 11:15 ZEU 255

Nonlinear dielectric spectroscopy in supercooled liquids — Peter Lunkenheimer[1], Marion Michl[1], Thomas Bauer[1], Francois Ladieu[2], Samuel Albert[2], and •Alois Loidl[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]SPEC, CEA, CNRS, University Paris-Saclay, France

We summarize the recent experimental status in non-linear dielectric spectroscopy on supercooled liquids. Nonlinearity can be measured by comparing the complex dielectric constants of high- and low-field permittivities [1] or by the determination of the higher harmonics of the permittivity [2]. Performing high-precision nonlinear dielectric experiments on glycerol and propylene carbonate, we find experimental evidence for growing cooperativity, implying clusters containing correlated molecules on approaching the glass transition. We were able to demonstrate that the number of dynamically correlated particles increases in much the same way as the effective energy barrier, [1] as predicted fifty years ago by Adam and Gibbs. By comparing third and fifth order susceptibilities, we again document the increase of amorphous order on decreasing temperatures. Moreover, we were able to determine the fractal dimension of these growing clusters. We find that they are compact and thus the glass transition can be regarded as a critical phenomenon, different from canonical phase transitions [3].

[1] Th. Bauer *et al.*, Phys. Rev. Lett. **110**, 107602 (2013).
[2] Th. Bauer *et al.*, Phys. Rev. Lett. **111**, 225702 (2013).
[3] S. Albert *et al.*, Science **352**, 1308 (2016).

15 min break

CPP 37.6 Wed 12:00 ZEU 255

Dynamics of Ethanol/Water mixtures studied by Dielectric spectroscopy — •Alexander Matt, Laura Vietze, and Bernd Stühn — Institut für Festkörperphysik, Technische Universität Darmstadt, D-64289, Germany

Water and alcohol mixtures have been an important part in studying the hydrogen bond network in water and the influence of guest molecules on the network. Since Ethanol is soluble in water at all concentrations it is well suited to act as a disturbance to the water network. In this work we use Ethanol, because of it is structural similarity to Poly(ethylene glycol), the only polyether soluble in water.

Ethanol and water mixtures form an eutectic system [1]. We use Differential Scanning Calorimetry in order to observe melting processes as well as glass transition temperatures. This method allows us to determine the eutectic phase diagram. In order to study the dynamics above, below and at phase transition temperatures Broadband Dielectric Spectroscopy is used. Measuring in the high frequency range between 200 MHz and 50 GHz both pure water and pure alcohol dynamics can be investigated [2] as well as their interplay. Results show, that adding small amounts of alcohol to water slows down the water dynamics and that the interaction between the Ethanol molecules has an influence as well. The results of both measurement techniques are compared and used to understand the influence of temperature and Ethanol concentration on the mixture. [1] K. Takaizumi et. al., J. Solution Chem. 26, 927(1997) [2] R. Böhmer et. al., Physics Report 545, 125(2014)

CPP 37.7 Wed 12:15 ZEU 255

^{1}H NMR at Larmor frequencies down to 3 Hz by means of Field-Cycling techniques — •Benjamin Kresse[1], Manuel Becher[1], Alexei F. Privalov[1], Marius Hofmann[2], Ernst A. Rössler[2], Michael Vogel[1], and Franz Fujara[1] — [1]Institut für Festkörperphysik, TU Darmstadt, Hochschulstr. 6, 64289 Darmstadt, Germany — [2]Experimentalphysik II, Universität Bayreuth, 95440 Bayreuth, Germany

Field-Cycling (FC) NMR traces spectral densities of molecular or ionic motions by measuring the spin-lattice relaxation dispersion in a broad range of Larmor frequencies. By rapidly switching the magnetic field from a high polarization field down to a small evolution field the relaxation process can be tracked in ultra low magnetic fields by switching up to a high detection field for signal acquisition. This contribution briefly deals with the technical part of our home built FC relaxometer and focuses on experiments at ultra low Larmor frequencies down to about 3 Hz demonstrating the performance of FC NMR. Several low field experiments are presented: Larmor precession about tilted evolution fields, simultaneous measurements of the Larmor frequency and the spin-lattice relaxation [B. Kresse, A. F. Privalov, A. Herrmann, M. Hofmann, E. A. Rössler, F. Fujara; Solid State NMR 59-60 (2014) 45-47.] as well as the irradiation of oscillating transversal magnetic field pulses as a novel method for field calibration in low field FC NMR. The potential of low field FC is exemplified by the ^{1}H relaxation dispersion of water at low frequencies stemming from the slow proton exchange process.

CPP 37.8 Wed 12:30 ZEU 255

Incipient Ferroelectricity of Nano-Confined Water Molecules — Boris Gorshunov[1,2], Elena Zhukova[1,2], Mikhail Belyanchikov[2], Victor Thomas[3], Pavel Tomas[4], Maxim Savinov[5], Christelle Kadlec[5], and •Martin Dressel[1] — [1]1. Phys. Inst., Univ. Stuttgart, Germany — [2]MIPT, Dolgoprudny, Russia — [3]Inst. Geol. Mineral., Novosibirsk, Russia — [4]Indep. Univ. Moscow, Russia — [5]Czech Acad. Sci., Praha, Czech Republic

Although H_2O molecules exhibit an extremely large electrical dipole moment, neither liquid water nor ice are ferroelectric since short-range hydrogen bonds screen the long-range intermolecular dipole-dipole coupling. The situation changes drastically when water is confined on the nanoscale. Though theoretically predicted and simulated, the H_2O ferroelectric ordering has never been clearly observed experimentally.

We have placed H_2O in the matrix of a beryl crystal lattice where the single water molecules are separated far enough from each other to avoid hydrogen bonds, but close enough to retain the dipole-dipole interaction. Using broad-band dielectric spectroscopy we demonstrate incipient ferroelectricity within the ensemble of interacting water molecules: on cooling, the static permittivity increases according to the Curie-Weiss law as a ferroelectric soft mode develops in the THz frequency range. At low temperatures quantum fluctuations eventually suppress the ferroelectric phase transition and lead to a saturation of the soft mode parameters and of the static permittivity. We model the results with the approach of a ferroelectric orientational phase transition.

CPP 37.9 Wed 12:45 ZEU 255

Dielectric response in organic solvents: polarizable force field models for dichloroethane — •Jakob Timmermann, Zhu Liu, Christoph Scheurer, and Karsten Reuter — Theoretische Chemie, TU München, Lichtenbergstr. 4, 85748 Garching bei München, Germany

Liquid/liquid interfaces between two immiscible fluids, e.g. between an aqueous phase and an organic solvent, have been considered as promising environments to embed catalytically active nano-particles into [1]. For most predictive-quality first-principles electronic structure calculations investigating catalytic processes in such systems, it is crucial to efficiently, yet accurately, model the interfacial region. One common approach is to explicitly simulate the solvent region via molecular dynamics (MD), approximating the Coulomb interaction among solvent molecules, as well as the electrostatic QM embedding via static, atom-centred partial charges. While these models are reported to yield sufficiently accurate results for isotropic bulk fluids, the approach is most likely insufficient to fully describe the anisotropic character of and electronic polarization at the interface. Based on the Drude oscillator model [2, 3] we developed a polarizable model of 1,2-dichloroethane (DCE) and analysed its performance for several macroscopic properties including the dielectric permittivity in comparison to our recently reparametrized non-polarizable 1,2-DCE model.

[1] Ge et al., PNAS 109 (2012), 11558.
[2] Lamoureux and Roux, J. Chem. Phys. 119 (2003), 3025.
[3] Dequidt et al., J. Chem. Inf. Model. 56 (2016), 260.

CPP 38: Fundamentals of Perovskite Photovoltaics V (joint session CPP/DS/HL)

Time: Wednesday 10:15–12:45 Location: ZEU 250

Invited Talk CPP 38.1 Wed 10:15 ZEU 250

Light-induced degradation of methylammonium and formamidinium PbI3 perovskites — •Norbert H. Nickel, Felix Lang, Victor V. Brus, and Jörg Rappich — Helmholtz-Zentrum Berlin für Materialien und Energie, Institut für Silizium Photovoltaik, Kekuléstr. 5, 12489 Berlin

We investigate the stability of methylammonium (CH3NH3+ - MA) and formamidinium (HC(NH2)2+ - FM) lead iodide perovskite films using visible and ultra violet light in oxygen atmosphere and in vacuum. Insight into the degradation mechanisms was obtained from in-situ Fourier-transform infrared absorption (FT-IR), photoluminescence, and gas effusion measurements. We revisited the light-induced degradation of MAPbI3 in the presence of oxygen. Illumination in O2 atmosphere results in a swift degradation. Isotope experiments clearly show that O2 acts as a catalyst decomposing MA ions into CH3NH2 and hydrogen. In case of FMPbI3 perovskites illumination in the presence of O2 results in a more complex reaction; decomposition of the FM ions occurs at the N-C-N bonds and as a result CO2 and C = O molecules are formed that rapidly diffuse out of the crystalline lattice.

In addition, we present experimental evidence of a hitherto unknown but fundamental degradation mechanism of MAPbI3 and FMPbI3 perovskite layers due to exposure to visible and ultra violet light. This degradation mechanism does not require the presence of oxygen or other constituents. Our data indicate that the molecular orbitals of the organic ions are not in resonance with the energy bands of the perovskite.

CPP 38.2 Wed 10:45 ZEU 250

Degradation Studies of Methylammonium Lead Iodide under Controlled Exposure to Oxygen and Light — •Paul Fassl, Qing Sun, David Becker-Koch, Alexandra Bausch, and Yana Vaynzof — Kirchhoff-Institute for Physics / Centre for Advanced Materials, Heidelberg University, Germany.

Despite the remarkable increase in the power conversion efficiency of hybrid organometal-halide perovskite solar cells reaching 22% to date, the low environmental stability of the material remains only partly understood. While the instability of methylammonium lead iodide (CH3NH3PbI3) in humid atmospheres has been studied experimentally as well as theoretically, degradation in the presence of oxygen and light has just recently been reported.

In this work, planar pinhole-free perovskite films are degraded under dry conditions with precisely controlled exposure to various oxygen levels and simulated sunlight using our environmental stability testing rig and then characterized by multiple techniques such as XPS, PDS, PL, AFM and SEM. These results are then correlated to the efficiency decay of photovoltaic devices (ITO/PEDOT:PSS/CH3NH3PbI3/PCBM/BCP/Ag), where the bare perovskite film has been first degraded under identical conditions.

Our results show that exposure to oxygen and light is one of the major reasons for the fast degradation of unencapsulated perovskite solar cells at ambient conditions and that the morphology and defect density of the pristine perovskite film has a considerable impact on the rate of degradation.

CPP 38.3 Wed 11:00 ZEU 250

Real-Time Observation of Iodide Ion Migration in Methylammonium Lead Halide Perovskites — •Cheng Li[1], Antonio Guerrero[2], Yu Zhong[1], Anna Gräser[1], Carlos Andres Melo Luna[3], Jürgen Köhler[3], Juan Bisquert[2], Richard Hildner[3], and Sven Huettner[1] — [1]Macromolecular Chemistry I, Universität Bayreuth, Universitätstr. 30, 95447 Bayreuth, Germany — [2]Institute of Advanced Materials (INAM), Universitat Jaume I, 12006 Castell, Spain — [3]Experimental Physics IV and Bayreuth Institute of Macromolecular Research, Universität Bayreuth, Universitätstr. 30, 95447 Bayreuth, Germany

To investigate the origin of current-voltage (J-V) hysteresis characteristic in perovskite solar cells (PSC), we utilize correlated time-resolved photoluminescence (PL) microscopy and impedance spectroscopy (IS) on perovskite films to in-situ investigate both the spatial and temporal evolution of these PL inactive areas under external optical/electrical fields. We attribute the formation of PL inactive domains to the migration and accumulation of iodine ions under external electrical fields. Furthermore, we fabricate and characterize PSC incorporating phenyl-C61-butyric acid methyl ester (PCBM) and PCBM polymer to investigate the influence of diffusions of PCBM molecules on the hysteretic behavior. Following that, the step-wise temperature dependent J-V measurement demonstrates the reduction of migration with the aid of PCBM molecules. Hence, it is proposed that the elimination/alleviation of J-V curve hysteresis is ascribed to the diffusion of PCBM molecules, which passivate the iodide related defects.

CPP 38.4 Wed 11:15 ZEU 250

Polarization of Methylammonium Lead Halide Perovskite Films on Microstructured Arrays — •Martina Stumpp[1,3], Raffael Ruess[1,3], Jan Muessener[2,3], and Derck Schlettwein[1,3] — [1]Justus-Liebig-University Giessen, Institute of Applied Physics — [2]Justus-Liebig-University Giessen, 1st Physics Institute — [3]Justus-Liebig-University Giessen, Laboratory for Materials Science

Despite the great advances of methylammonium lead halide perovskites in photovoltaics, many properties such as the I-V hysteresis of such films are not fully understood and, therefore, need detailed investigation. In the current study, $CH_3NH_3PbI_3$ and $CH_3NH_3Pb(I_{3-x}Cl_x)_3$ films were prepared on microstructured gold or platinum electrode arrays on SiO_2/Si wafers in order to use symmetric contacts and widely inert substrates. The perovskite films were poled with high voltages and the current was measured under variation of ambient parameters and analyzed in detail. Following the poling of the samples, voltage sweeps were performed. The I-V characteristics during these sweeps showed clearly that the perovskite films were polarized and that the polarization had a persistent character. Additionally, different hysteresis characteristics were observed. The origin of regular and inverted characteristics will be discussed.

15 min break

CPP 38.5 Wed 11:45 ZEU 250

Characterization of the perovskite solar cells containing atomic layer deposited Al_2O_3 buffer layer. — •Małgorzata Kot[1], Konrad Wojciechowski[2], Henry Snaith[2], and Dieter Schmeisser[1] — [1]BTU Cottbus-Senftenberg, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany — [2]Clarendon Laboratory, University of Oxford, Parks Road, Oxford, OX13PU, UK

Hybrid perovskites have potential to overcome performance limits of the current solar cell technologies and achieve low cost and high versatility. Nonetheless, they are prone to degradation in presence of moisture within a couple of hours or days. In this work, we use the atomic layer deposition (ALD) of Al_2O_3 on the $CH_3NH_3PbI_3$ perovskite at room temperature in order to verify if this thin ALD layer may protect the perovskite film against moisture degradation and to check the impact of the Al_2O_3 on the solar to power conversion efficiency (PCE). Depth profiling X-ray photoelectron spectroscopy study shows that the ALD precursors are chemically active only at the perovskite surface and the film bulk is not affected. The perovskite film coated with Al_2O_3 layer has enhanced moisture stability. Solar cells with a fresh-made $CH_3NH_3PbI_3$ perovskite film have shown PCE of 15.4%, while the one with 50 days aged perovskite only 6.1%. However, when the aged perovskite is covered with RT-ALD-Al_2O_3 the PCE value is clearly enhanced.[1]

[1] M. Kot et al., Room temperature ALD impact on efficiency, stability and surface properties in perovskite solar cells, ChemSusChem, acctepted.

CPP 38.6 Wed 12:00 ZEU 250

Influence of the grain size on electronic properties of methylammonium lead iodide — •Oleksandra Shargaieva, Felix Lang, Jörg Rappich, Thomas Dittrich, Bernd Rech, and Norbert Nickel — Helmholtz-Zentrum Berlin, Institute for Silicon Photovoltaics, Kekulestr. 5, D-12489 Berlin (Germany)

Recently, hybrid perovskites have drawn the attention of researchers due to huge potential as absorbers in photovoltaic devices. The biggest advantage of such materials is the ease of the preparation within low costs leading to highly efficient solar cells. However, the solution based processing often lacks a control over crystal quality of obtained material. Despite the numerous reports showed different methods to improve morphology of perovskite layer, the influence of microscopic structure on properties of the material is not fully understood.

In this work we present a new approach to tune the grain size of CH3NH3PbI3 perovskite from 150 to 1000 nm with about 100 nm step. The new method is based on solid-phase recrystallization and provides a reliable way to control the grain size and hence, systematically study the influence of the grain size on optical and electrical properties of the material. The recrystallized perovskite layers were characterized using photoluminescence spectroscopy and surface photovoltage measurements. The recrystallized samples demonstrated a pronounce increase of the PL intensity due to lower defect density in treated material. Furthermore, our study showed a direct correlation between grain size and the transport length, L, with the maximum value of 900 nm.

CPP 38.7 Wed 12:15 ZEU 250

Investigation of novel material systems for hybrid photovoltaics - alternatives for the paradigm — •Nuri Hohn[1], Mike Boone[2], Eric Rivard[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]University of Alberta, Department of Chemistry, Edmonton, Alberta, Canada

Organic materials have been found to offer various, promising advantages for photovoltaic (PV) devices like flexibility and the potential of low-cost/large scale production. Hybrid devices combine these advantages with the chemical/physical stability of inorganic materials and, thus, overcome the issue of limited lifetimes of purely organic cells. Poly(styrene-block-ethylene oxide) templated sol-gel chemistry is used to synthesize high surface-to-volume ratio, mesoporous titania thin films, which allows for precise structure control and an increased amount of interface. The n-type, electron conducting titania thin film serves as a basis for novel organic material studies. The studies aim to introduce new material combinations to the field of hybrid PV and to open up pathways for enhanced efficiency in terms of energy conversion and band alignment. Thin film spectral absorption characterization is carried out via UV/Vis measurements. Furthermore, morphological characterization is realized via SEM and XRD to address to surface structure and the crystallinity of the material.

CPP 38.8 Wed 12:30 ZEU 250

Water-processed hybrid solar cells: deposition of the active layer with vertical composition gradient — •Volker Körstgens[1], Florian Buschek[1], Martin Wörle[2], Hristo Iglev[2], Wiebke Ohm[3], Stephan V. Roth[3], Reinhard Kienberger[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]TU München, Physik-Department, LS Laser- und Röntgenphysik, James-Franck-Str. 1, 85748 Garching — [3]DESY, Notkestr. 85, 22607 Hamburg

Particular environmentally friendly processing of hybrid solar cells with the solvent water is feasible with an active layer consisting of laser-ablated titania and a water-soluble polythiophene [1]. One way to optimize conversion efficiencies of these devices is the introduction of a vertical compositional gradient of the two components of the active layer. Dip-coating and spray-coating have been utilized as techniques which are suitable for the cost-effective preparation of hybrid photovoltaics. We followed the development of the morphology during spray deposition in situ with high spatial and temporal resolution. The mesoscale was probed with GISAXS and the crystallinity of the polymer and the inorganic component was probed with GIWAXS. The changes of the morphology and the influence on photovoltaic performance with the introduction of a compositional gradient are discussed. [1] Körstgens et al., Nanoscale 7, 2900 (2015).

CPP 39: Organic Photovoltaics and Electronics II (joint session CPP/DS/HL, organized by HL)

Time: Wednesday 14:45–17:45 Location: POT 81

CPP 39.1 Wed 14:45 POT 81

singlet fission process of organic molecules attached to neon clusters — •sharareh izadnia, aaron laforge, and frank stienkemeier — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

Charge and excitation transfer along with the corresponding decay and loss mechanism are fundamental aspects in light harvesting, organic photovoltaics, and optoelectronic devices.

In particular, singlet fission is a unique decay mechanism where a molecule excited to its singlet state can partially transfer its energy to a neighboring ground state molecule, and thereby create two molecules excited to a triplet state. As such, singlet fission can increase the efficiency of organic electronics and photovoltaic by creating multiple charge carriers from one single photon. Here, we report a systematic study of acene complexes attached to the surface of neon clusters. Depending on the system parameters, singlet fission and other lifetime reduction mechanisms are observed.

CPP 39.2 Wed 15:00 POT 81

Novel Organic NIR Detector Class Based on Charge-Transfer Absorption — •Bernhard Siegmund, Andreas Mischok, Johannes Benduhn, Olaf Zeika, Sascha Ullbrich, Frederik Nehm, Donato Spoltore, Hartmut Fröb, Christian Körner, Karl Leo, and Koen Vandewal — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden, Dresden, Germany

Blending two organic species on a molecular level can introduce interfacial states which allow to absorb far below their optical gap. Although such intermolecular charge-transfer (CT) states form an important recombination path in organic solar cells, their near-infrared (NIR) absorption properties have been unused for photo-sensitive devices up to now. In this presentation, we disclose a new resonant optical cavity device architecture enabling NIR photodetection by means of efficient CT absorption. We demonstrate tunable detection wavelengths between 810nm and 1550nm with a single material blend, far below the optical gap of both donor and acceptor. The combination of spectral narrowband detection and broad tunability make this novel, flexible and potentially visibly transparent device principle highly suitable for integrated low cost spectroscopic NIR photodetection.

CPP 39.3 Wed 15:15 POT 81

Revealing the loss mechanisms in ZnO/organic hybrid solar cells — •Moritz Eyer[1], Sebastian Kickhöfel[2], Johannes Frisch[2], Sergey Sadofev[1], Joachim Puls[1], Norbert Koch[1], Emil List-Kratochvil[2], and Sylke Blumstengel[2] — [1]Institut für Physik, Humboldt-Universität zu Berlin — [2]Inst. f. Physik, Inst. f. Chemie und IRIS Adlershof, Humboldt-Universität zu Berlin

In order to study the losses of ZnO/organic hybrid photovoltaic devices a model system of ZnMgO and poly(3-hexylthiophene) (P3HT) is introduced. It allows tuning the interface band gap energy between the ZnMgO conduction band minimum and the P3HT HOMO systematically by varying the Mg content in the inorganic component. This enables a profound study of charge separation and recombination processes at the interface of inorganic/organic hybrid heterojunctions.

Prior to full charge separation electron and hole on opposite sides of the interface form hybrid charge transfer excitons (HCTX) bound by Coulomb interaction [1]. Electroluminescence measurements in the near IR spectral range confirm the existence of HCTX and yield valuable information of their physical properties. Temperature dependent photovoltaic measurements provide the necessary information to understand the charge separation process and its influence on the parameters defining the performance of a photovoltaic device. A detailed study of the interface energetics allows quantifying the recombination losses of inorganic/organic hybrid heterojunctions in order to fully exploit their potential in solar energy.

[1] M. Eyer et. al. Appl. Phys. Lett. 107, 221602 (2015).

CPP 39.4 Wed 15:30 POT 81

Silver nanowires and polymer based transparent electrodes for Organic solar cells — •Yoonseok Park, Ludwig Bormann, Koen Vandewal, and Karl Leo — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden, Germany

Organic photovoltaics (OPV) are prospective candidates for future renewable energy production because of their potential scalability, low cost, and flexibility. For establishing flexible organic devices, a highly transparent, conductive and flexible electrode is required, replacing ITO which is brittle and requires high temperature processes. Many alternative materials such as conductive polymers, graphene, and metal nanowires have been studied. Among these, metal nanowires, especially silver nanowire (AgNW) networks, show outstanding flexibility, conductivity, and transparency. However, AgNW network electrodes have a few basic problems: (i) a poor electrical contact between wires, resulting in a low conductivity, (ii) overlapping wires cause roughness, often resulting in electrical shorting of devices and (iii) open spaces between wires can be in the range of square micrometers. In this study, highly conductive PEDOT:PSS has been deposited on AgNW electrodes to form conductive bridges between the open spaces and to smoothen the sharp points of the network. The maximum process temperature is 120 °C. OPV cells using these AgNW / PEDOT:PSS transparent electrodes exhibit power conversion efficiencies up to 7.15%. Moreover, OPV devices on PET substrates with an alumina encapsulation and barrier adhesive show excellent mechanical flexibility.

CPP 39.5 Wed 15:45 POT 81

Three-dimensional graphene-based electrodes for asymmetric supercapacitors — •Maximilian von Seckendorff[1], Simon Drieschner[1], Jörg Wohlketzetter[1], Jose A. Garrido[2], and Martin Stutzmann[1] — [1]Walter Schottky Institut und Physik-Department, Technische Universität München, Garching, Germany — [2]The Barcelona Institute of Science and Technology, Bellaterra, Spain

Three-dimensional (3D) graphene-based structures combine the outstanding physical and chemical properties of graphene such as high conductivity, mechanical stability and chemical inertness with a high surface-to-volume ratio, making them highly promising for energy storage applications in supercapacitors. Here we demonstrate the fabrication of 3D graphene-based electrodes by chemical vapor deposition using sintered copper particles and electrodeposited nickel/copper alloys as catalytic metal substrates. After selective wet chemical etching of the metal scaffold, a freestanding graphene foam of high structural quality as confirmed by Raman spectroscopy is obtained. In an asymmetric supercapacitor, this graphene foam is used as the cathode and is combined with a graphene foam coated with pseudocapacitive elements such as manganese dioxide as the anode. This combination results in an extended electrochemical potential window above 1.5 V and, therefore, a higher energy density ($>$ 5 Wh/kg) compared to symmetric supercapacitors. The electrochemical performance of this asymmetric capacitor is investigated by cyclic voltammetry, electrochemical impedance spectroscopy, and charge-discharge-measurements and confirms its great potential for energy storage applications.

Coffee Break

CPP 39.6 Wed 16:30 POT 81

Semitransparent Electrodes for Evaporated Small Molecule Organic Solar Cells — •Dhriti Sundar Ghosh and Karl Leo — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), TU Dresden

Transparent Electrodes are key in novel flexible devices. We report a highly efficient microcavity assisted small molecule organic solar cell (SM-OSC), containing an indium-free semitransparent TiO2(30nm)/Ag 9nm based transparent electrode with average visible transmittance of 66.7% and sheet resistance of 6.3 Ohm/sq. The electrode also consisted of a wetting layer of polyethyleneimine which promotes the growth of ultrasmooth, and highly conductive Ag films even at very low thicknesses. The role of high index TiO2 undercoat layer is investigated in detail by optical simulations and is shown to enhance the microcavity effect, leading to increased light coupling into the photoactive layer. With comparable photocurrent, and high fill-factor values owing to much better electrical properties, the semitransparent electrode based SM-OSC outperforms the state-of-art indium tin oxide (ITO) based reference device with photon conversion efficiency of 8.1% compared to 7.7% despite having lower transmittance (~21%) relative to ITO. This work demonstrates that a properly designed semitransparent TE is a promising alternative to ITO and can lead to more efficient photovoltaic devices.

CPP 39.7 Wed 16:45 POT 81

Intereference-induced thermoelectric effects in topological states of matter — •Flavio Ronetti[1,2], Luca Vannucci[1,2], Giacomo Dolcetto[3], Matteo Carrega[4], and Maura Sassetti[1,2] — [1]Dipartimento di Fisica, Università di Genova,Via Dodecaneso 33, 16146, Genova, Italy. — [2]CNR-SPIN, Via Dodecaneso 33, 16146, Genova, Italy. — [3]Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg. — [4]NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, I-56127 Pisa, Italy.

In topological states of matter, such as edge states of quantum Hall systems and two-dimensional topological insulators, protection from backscattering guarantees phase-coherent ballistic transport, allowing for the observation of quantum interference effects. Intriguing thermoelectric properties can be achieved by exploiting the phase-coherent edge states of two quantum Hall systems coupled by tunnelling region. Considering a multiple quantum point contacts geometry, interference paths effectively break the electron-hole symmetry. Therefore, when the systems are driven out of equilibrium by a thermal gradient, a thermoelectric charge current can be induced. Correspondingly, an interference pattern in the heat current is predicted. In the case of two-dimensional topological insulators, the presence of spin degree of freedom give rise to a rich tunnelling dynamics. In a double quantum point contact geometry, the effective transmission related to spin-flipping processes acquires a functional dependence on energy in the interacting regime, thus generating a thermoelectric spin current in response to a thermal gradient.

CPP 39.8 Wed 17:00 POT 81

Organic thermoelectrics based on low-dimensional molecular metals — •Alexander Steeger[1], Florian Huewe[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Efficient recovery of waste heat by thermoelectric generators (TEGs) requires low-cost materials exhibiting high electrical conductivities σ and Seebeck coefficients S, but low thermal conductivities κ. The suitability of a given material for thermoelectric applications is quantified by the dimensionless figure of merit $zT = \sigma S^2 T/\kappa$. In this contribution, we propose crystalline low-dimensional molecular metals as an alternative class of organic thermoelectric materials combining the advantages of low weight, chemical variety, sustainability, high charge carrier mobility and reduced electronic dimensionality with the availability of p- and n-type conductors. For the first time, we determined all physical quantities contributing to zT on exclusively one single crystal sample of p-type $\mathrm{TTT_2I_3}$ and n-type $\mathrm{(DMe\text{-}DCNQI)_2Cu}$, revealing high power factors and promising figures of merit surpassing $zT \geq 0.15$ below 40 K. The thermoelectric performance of low-dimensional metals is affirmed by the power output per active area of a prototypical all-organic TEG reaching values of ~$\mathrm{mW/cm^2}$ and could be further increased by taking full control over the amount of charge-transfer and band filling. Financial support by the DFG (Project No. PF385/6-1) and the FP7 (H2ESOT, Project No. 308768) of the European Commission is gratefully acknowledged.

CPP 39.9 Wed 17:15 POT 81

Ag-segregation at dislocations and grain boundaries in annealed PbTe thermoelectric materials studied by atom probe tomography — •Yuan Yu[1], Oana Cojocaru-Mirédin[1], Yaron Amouyal[2], Ariel Sheskin[2], and Matthias Wuttig[1] — [1]I. Physikalisches Institut (IA), RWTH Aachen, 52074, Aachen, Germany — [2]Technion-Israel Institute of Technology, 32000 Haifa, Israel

PbTe-based alloys play a significant role in thermoelectric (TE) applications. The figure-of-merit, ZT, of standard PbTe is near 1, whereas for PbTe alloys doped with Sr, Na, K, and Ag, the ZT factors are larger than 2. The large enhancement of ZT values mainly benefits from the elemental doping-induced band modification and nano-precipitation. However, the effects of these dopants on the TE properties is still not well understood mainly due to the difficulty to track the impurity redistribution in 3D with traditional characterization techniques. Here, we investigated the distribution of Ag in PbTe TE material using 3D atom probe tomography. We clearly find that the Ag is prone to form platelet-like nanostructures with diameters of ~15 nm and thickness of ~3 nm in the as-quenched state. After annealing at 380 °C for 48 h, these platelet-like nanostructures dissolve in the matrix, leading to a Ag-supersaturated matrix. Thus, the Ag tends to segregate at the dislocations and grain boundaries. These Ag-decorated dislocations and grain boundaries as well as the remaining stable Ag-rich nanoprecipitates are believed to influence the electron and phonon transport processes. Our results can help to better tailor the structures and provide more information for the theoretical calculation.

CPP 39.10 Wed 17:30 POT 81

Potassium Prussian Blue Nanoparticles: A Low-cost Cathode Material for Potassium-ion Batteries — •Yang Xu, Min Zhou, Liying Liang, and Yong Lei — Institute für Physics & IMN MacroNano (ZIK), Technische Universität Ilmenau, Ilmenau 98693, Germany

Potassium-ion batteries (KIBs) in organic electrolytes hold great promise owing to the abundance of potassium, close redox potential to lithium, and similar electrochemistry with lithium system. Investigations of KIB cathodes have been scarcely reported so far. We for the first time report hydrated potassium Prussian blue K0.220Fe[Fe(CN)6]0.805 nanoparticles as a potential cathode material. The cathode exhibits a high discharge voltage of 3.1~3.4 V, high reversible capacity of 73.2 mAh g-1, and great cyclability with a very small capacity decay rate of ~0.09% per cycle. Electrochemical reaction mechanism analysis identifies the carbon-coordinated FeIII/FeII couple as redox-active site and proves structural stability of the cathode during charge/discharge. Furthermore, we present a KIB full-cell by coupling the nanoparticles with commercial carbon materials. The full-cell delivers a capacity of 68.5 mAh g-1 at 100 mA g-1 and retains 93.4% of the capacity after 50 cycles. Considering the low cost and material sustainability, this work may trigger future attention on rechargeable KIBs.

Reference

C. Zhang, Y. Xu, M. Zhou, L. Liang, H. Dong, M. Wu, Y. Yang, Y. Lei, Adv. Funct. Mater. 2016, DOI: 10.1002/adfm.201604307.

CPP 40: Focus: Polymer Crystallization - from Model Systems to New Materials II

Time: Wednesday 15:00–18:15 Location: ZEU 222

Invited Talk CPP 40.1 Wed 15:00 ZEU 222

Architectural Engineering of Semi-Crystalline Elastomers — •Sergei Sheiko — University of North Carolina at Chapel Hill, USA

Molecular assembling, including polymer crystallization and hydrogen bonding, is an effective tool for creating moldable and dynamic networks with unique physical properties such as reversible and time-programmable shape memory. Unlike linear polymer melts, the crystallization process of polymer networks is guided by the network architecture described by the mesh dimensions and branching of the network strands. Synthetic control of architectural parameters allows for accurate variation of the degree of crystallinity, physical crosslink density, and crosslink functionality. We will discuss different examples of the architectural control of structure-property correlations for different types of polymer networks including super-soft and super-elastic brush-like elastomers and linear-chain elastomers that display reversible shapeshifting.

CPP 40.2 Wed 15:30 ZEU 222

Thermally induced shape-memory actuators on the basis of crosslinked poly(ϵ-caprolactone) — •Oleksandr Dolynchuk[1], Igor Kolesov[2], Dieter Jehnichen[1], Hans-Joachim Radusch[2], and Jens-Uwe Sommer[1,3] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Germany — [2]Martin Luther University Halle-Wittenberg, Center of Engineering Sciences, Germany — [3]Technische Universität Dresden, Institute for Theoretical Physics, Germany

Polymer materials capable of active motion in response to external stimuli have an outstanding potential for numerous applications from space engineering to smart bioimplants, nanostructures etc. The evolution of the thermally induced invertible shape-memory effect (SME) under constant load was investigated in crosslinked linear poly(ϵ-caprolactone) (PCL). The viscoelastic and thermal properties as well as morphology, size, and orientation of crystals in PCL networks were analyzed as well. In addition, PCL with the highest achieved crosslink density revealed remarkable invertible actuation under stress-free conditions. The oriented growth of crystals was found to be the origin of the invertible SME under and without load. The mean field approach was used to calculate the free energy change during non-isothermal crystallization of PCL networks under load, whereby the possible morphology and orientation of crystals were analyzed. The analytical results on the nanocrystalline structure along with fitting curves of strain vs. temperature, which were got by modeling the SME in PCL under load, correspond well to the experimental outcomes.

CPP 40.3 Wed 15:45 ZEU 222

Molecular order in strain-recrystallized Poly-Caprolactone — •Wilhelm Kossack[1], Anne Seidlitz[2], Thomas Thurn-Albrecht[2], and Friedrich Kremer[1] — [1]Universität Leipzig, Molecular Physics, 04103 Leipzig, Germany — [2]Universität Halle-Wittenberg, Experimentelle Polymerphysik, 06120 Halle/Saale, Germany

Biaxial order in free standing films of Poly-ϵ-Caprolactone is induced by plastic deformation and concomitant re-crystallization. The three-dimensional orientation distribution is studied by Infrared transition moment orientational analysis (IR-TMOA) and X-ray diffraction (pole figure) measurements. The former method senses the alignment of *amorphous moieties and crystal directions* (*eg.* [001]), whereas the latter technique reveals the order of the (200)- and (110)-crystal-planes. The main chains of the polymers are aligned with the stretching direction, leading to a strong uniaxial order with an order parameter (Hermans orientation function) of $S_{xx} \approx 0.9 \pm 0.1$ for the crystalline $\underline{c}$-axes ([001]). The amorphous polymer backbones exhibit a lower, $S_{xx} < 0.7$, slightly biaxial order. Furthermore, changes in the XRD-diffractograms and IR-spectra upon stretching indicate strained lamellar crystallites and a reduction of crystallinity upon stretching.

CPP 40.4 Wed 16:00 ZEU 222

Aligned crystallization within a single gyroid network of a semicrystalline triblock terpolymer — •James A. Dolan[1], Raphael Dehmel[1], Bodo D. Wilts[2], Alessandro Sepe[2], Yibei Gu[3], Timothy D. Wilkinson[1], Jeremy J. Baumberg[1], Ulrich Wiesner[3], Ullrich Steiner[2], and Ilja Gunkel[2] — [1]University of Cambridge, Cambridge, UK — [2]Adolphe Merkle Institute, Fribourg, CH — [3]Cornell University, Ithaca, NY, USA

Semicrystalline block copolymers are an interesting model system for studying the crystallization of polymers under nanoscale confinement. Confined crystallization takes place if the crystallization temperature of the semicrystalline block is lower than the glass transition temperature of the amorphous block. This confinement is often found to induce aligned crystallization. In this work, the crystallization of semicrystalline poly(ethylene oxide) (PEO) confined within a single gyroid morphology was studied in solvent-annealed polyisoprene-*b*-polystyrene-*b*-poly(ethylene oxide) (ISO) triblock terpolymer films by means of GISAXS, GIWAXS, SEM, and optical microscopy. PEO is shown to crystallize preferentially in the direction of the least tortuous pathways of the gyroid, leading to a preferential alignment of the PEO crystallites within the self-assembled morphology. Strikingly, this gives rise to an optical birefringence of individual gyroid domains that allows mapping of the grain structure in self-assembled ISO films by means of optical microscopy.

15 min break

Invited Talk CPP 40.5 Wed 16:30 ZEU 222

Chain Trajectory of Semicrystalline Polymers as Revealed by Solid-State NMR Spectroscopy — •Toshikazu Miyoshi — The University of Akron, Department of Polymer Science, Akron OH, USA

Over the last half century, chain-folding structure of semicrystalline polymers has been debated in polymer science. Recently, 13C-13C double quantum (DQ) NMR spectroscopy combined with 13C selective isotope labeling has been developed to investigate re-entrance sites of the folded chains, mean values of adjacent re-entry number <n> and fraction <F> of semicrystalline polymers. This viewpoint highlights the versatile approaches using NMR and isotope labeling for revealing i) chain trajectory in melt- and solution-grown crystals, ii) conformation of the folded chains in single crystals, iii) self-folding in the early stage of crystallization, and iv) unfolding of the folded chains under stretching.

CPP 40.6 Wed 17:00 ZEU 222

Creating micrometer-high stacks of correlated lamellar crystals of precision polyethylene by self-induced nucleation — •Sumit Majumder[1], Hanna Busch[2], Purushottam Poudel[1], Stefan Mecking[2], and Günter Reiter[1] — [1]Experimental Polymer Physics, University of Freiburg — [2]Chair of Chemistry, University of Konstanz

Crystallizable polymers often form stacks of correlated lamellar crystals. Formation of such stacks of lamellae requires a mechanism of self-induced nucleation at the fold surface (H. Zhang et. al. Phys. Rev. Lett. 112, 237801, (2014)). However, in polymer thin films, scarce availability of polymers on the fold surface and a low nucleation probability in general typically limit the formation of such stacks of lamellar crystals. Here, we investigate the possibility of enhancing stacking of lamellar crystals in thin films by introducing precisely spaced bulky methyl-phosphonate groups along the backbone of polyethylene. Presence of these bulky side groups impose constraints on folding and eliminate the possibility of lamellar thickening. We present experimental observations indicating that the stacking mechanism can be controlled by film thickness, crystallization temperature and molecular weight.

CPP 40.7 Wed 17:15 ZEU 222

Interface-induced crystallization via prefreezing: A first-order prewetting transition — •Ann-Kristin Flieger, Martha Schulz, and Thomas Thurn-Albrecht — Experimental Polymer Physics, Institute of Physics, Martin Luther University Halle-Wittenberg, 06120 Halle, Germany

Prefreezing is a mechanism of surface-induced crystallization. In prefreezing a crystalline layer is formed at the interface of a solid substrate and the liquid phase already above the melting point. Wetting theory predicts a jump in thickness at the formation and a divergence upon approaching coexistence. However, the thickness of the prefreezing layer has not been experimentally measured so far.

We studied ultrathin films of Polycaprolactone during the crystallization on graphite. With AFM at high temperatures we observe prefreezing instead of heterogeneous nucleation. The corresponding crystalline layer is formed at a temperature above the bulk melting point. Similar observations were already made for polyethylene on graphite (A.-K. Löhmann et al., PNAS 49, 17368-17372 (2014)). In that case however, a direct measurement of the thickness of the prefreezing layer was not possible. Here, we show directly the finite thickness of the prefreezing layer for PCL. It forms with a thickness of a few nanometers which further increases during cooling. This observation demonstrates the transition is of first order, as expected for a prewetting transition.

The results prove that prefreezing can be described by common wetting theory. The studied system PCL-graphite is of importance for applications since graphitic materials are widely used as fillers for PCL.

CPP 40.8 Wed 17:30 ZEU 222

Interplay between the Relaxation of the Glass of Random L/D Lactide Copolymers and Homogeneous Crystal Nucleation: Evidence for Segregation of Chain Defects — •Christoph Schick[1,2] and Rene Androsch[3] — [1]Institute of Physics, University of Rostock, Albert-Einstein-Str. 23-24, 18051 Rostock — [2]Kazan Federal University, 18 Kremlyovskaya street, Kazan 420008, Russian Federation — [3]Center of Engineering Sciences, Martin Luther University Halle-Wittenberg, 06099 Halle/Saale

Random L isomer rich copolymers of poly(lactic acid) containing up to 4% D isomer co units have been cooled from the molten state to obtain glasses free of crystals and homogeneous crystal nuclei. The kinetics of enthalpy relaxation and the formation of homogeneous crystal nuclei have then been analyzed using fast scanning chip calorimetry. It has been found that the relaxation of the glass toward the structure/enthalpy of the supercooled liquid state is independent of the presence of D isomer co units in the chain. Formation of homogeneous crystal nuclei in the glassy state requires the completion of the relaxation of the glass. However, nucleation is increasingly delayed in the random copolymers with increasing D isomer chain defect concentration. The data show that the slower formation of homogeneous crystal nuclei in random L/D lactide copolymers, compared to the homopolymer, is not caused by different chain segment mobility in the glassy state but by the segregation of chain defects in this early stage of the crystallization process.

Invited Talk CPP 40.9 Wed 17:45 ZEU 222

The Role of Entanglement in Polymer Crystallization — •Chuanfu Luo — Max Planck Institute of Colloids and Interfaces, Am Mühlenberg 1 OT Golm, 14476 Potsdam, Germany

Polymer crystallization is one of the fundamental topics in polymer science. A deeper understanding of it has a great industrial importance as about 70% industrial plastics are of semicrystalline states. We carried out large scale MD simulations of polymer crystallization by using a coarse-grained poly(vinyl alcohol) (CG-PVA) model. We simulated different situations for linear polymers such as of dense melts, of concentrated solutions, under confinement of two walls, and under steady shears. We analyzed the entanglement states before the crystallization by using primitive path analysis (PPA) and its geometric analogue, the Z1 method. We found that the crystallization behavior is strongly related to the initial entanglement states. The crystalline stem length (d) is directly controlled by the initial entanglement length (N_e). The slow relaxation of entanglement state can be a major reason for the thermal memory effect. We found a roughly linear relation of $d = N_e/f$ for most cases, where f means an effective folding number with a value about 2.5 for dense melts or slightly larger for concentrated solutions. We propose that thickness selection in polymer crystallization is mainly restricted by the initial entanglement length. Our simulations may provide a novel approach to understand polymer crystallization at different situations.

CPP 41: Organic Electronics and Photovoltaics IV: OPV (joint session CPP/DS/HL, organized by CPP)

Time: Wednesday 15:00–18:30 Location: ZEU 260

Invited Talk CPP 41.1 Wed 15:00 ZEU 260

The role of incoherent hopping in the photogeneration of charges in organic semiconductors — •Anna Köhler — University of Bayreuth, 95400 Bayreuth, Germany

We demonstrate that efficient and nearly field-independent charge separation in organic planar heterojunction solar cells can be described by an incoherent hopping mechanism that can be modelled by kinetic Monte Carlo simulations that include the effect of on-chain delocalization. We address, first, the issue of differentiating between geminate and nongeminate recombination in solar cells.(Adv. Funct. Mater. 2016, DOI: 10.1002/adfm.201604906) We show that a reduced fill factor and the appearance of an s-shaped I-V curve even at low light intensities results from geminate recombination due to the back diffusion of holes toward their siblings at the donor-acceptor interface rather from to charge accumulation at the donor-acceptor interface. Second, we consider how optical excitation of C60 and PCBM contribute to the photogeneration of charge carriers. (J. Phys. Chem. C 2016 DOI: 10.1021/acs.jpcc.6b0847). We find that intrinsic photogeneration starts at a photon energy of about 2.25 eV, i.e., about 0.4 eV above S1. It originates from charge transfer type states that can autoionize incoherently via thermalization before relaxing to S1 state, in the spirit of Onsager's 1938 theory.

CPP 41.2 Wed 15:30 ZEU 260

Charge separation and recombination in PBTT-T/fullerene blends and solar devices — •Elisa Collado Fregoso[1], Jona Kurpiers[1], Samantha Hood[2], Ivan Kasal[2], James Durrant[3], and Dieter Neher[1] — [1]Institut für Physik und Astronomie, Potsdam University, Potsdam-Golm, Germany — [2]Centre for Quantum Computation and Communication Technology, The University of Queensland, Brisbane, Australia — [3]Centre for Plastic Electronics, Department of Chemistry, Imperial College London, UK

Organic solar cells, particularly polymer/fullerene solar cells, are an important area of scientific research on the generation of sustainable and renewable energy. However, further optimization of solar device efficiency is still needed to reach commercialization.

In this talk, the relationship between active layer nanostructure and charge separation and recombination kinetics in thin films and solar devices fabricated with mixtures of PBTT-T/fullerene will be established. Via a combined theoretical and experimental kinetic study using Transient absorption spectroscopy (TAS) and Time-delayed collection field (TDCF) we clearly establish the effect of an intermixed versus a more flat interface towards the separation of bound charges and charge recombination regimes. This is further correlated with device performance, thus showing the importance of careful blend nanostructure control.

CPP 41.3 Wed 15:45 ZEU 260

Electron Affinity and Charge Trapping in Ternary Fullerene-based Donor:Acceptor Films for Organic Photovoltaics — •Michael Auth[1], Michael Brendel[1], Andreas Sperlich[1], Stephan Väth[1], Jens Pflaum[1,2], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg

Fullerene materials for organic photovoltaics (OPV) are highly expensive, due to their elaborate purification. To determine if this step is necessary to a high degree, we investigate the influence of fullerene mixtures, i.e. unpurified fullerenes, in ternary OPV materials. As the molecule's electron affinity determines where charge carriers reside, it also determines if unintentional molecules act as trap sites. Since electron paramagnetic resonance (EPR) addresses localised charges, we investigate photo-induced charge transfer via EPR in correlation with solar cell parameters (V_{OC}, J_{SC}, PCE). For polymer-fullerene blends we used the conjugated polymers P3HT or PTB7, together with the soluble fullerene derivatives $PC_{70}BM$, $PC_{60}BM$ and $IC_{60}BA$. As comparison, we furthermore investigated solar cell absorbers made of various vacuum deposited mixtures of C_{70} and C_{60} fullerenes on top of Diindenoperylene (DIP). For all configurations we compare the redistribution of electrons in the fullerene phase with the corresponding stoichiometry to determine electron affinity differences. In conjunction with solar cell parameters we are then able to determine the influence of unpurified fullerenes upon OPV.

CPP 41.4 Wed 16:00 ZEU 260

Role of trapped and free charges on the recombination in a low band-gap organic solar cell — •Steffen Roland[1], Antonio Facchetti[2], and Dieter Neher[1] — [1]University of Potsdam, Institute of Physics and Astronomie, Potsdam, Germany — [2]Northwestern University, Department of Chemistry, Evanston, IL-USA

While the role of traps on the transport of photogenerated charges has been analyzed in detail in the literature, the effect of energetic disorder on the rate of non-geminate recombination is yet not very clear. In this talk a new comprehensive approach of how to treat recombination in energetically disordered organic solar cells is proposed. Charge extraction techniques are used to examine the recombination dynamics of a typical organic solar cell (PMDPP3T:PCBM) in detail. While temperature dependent steady-state charge extraction experiments predict a significant amount of trapped charges, it is found that the recombination current (J_R) is dominated by a bimolecular process. A model is introduced in which free charges (outside the Fermi-gap) that contribute to J_R are discriminated from trapped charges (inside the Fermi-gap), which do not contribute to J_R. The free charge carrier recombination coefficient is determined by time delayed collection field measurements and used to accurately fit the measured JV-characteristics over a wide range of light intensities. These results prove that in this system, although charges undergo trapping, the recombination current is dominated by free bimolecular carrier recombination. This work sheds new light on the influence of trapped charges on the recombination process, a topic that has yet remained controversial within the field.

CPP 41.5 Wed 16:15 ZEU 260

Recombination Dynamics and the Role of Space Charge Effects in Organic Photovoltaics — •Martin Stolterfoht[1], Ardalan Armin[2], Safa Shoaee[1], Bronson Philippa[3], Paul Meredith[2], and Dieter Neher[1] — [1]University of Potsdam, Potsdam-Golm, Germany — [2]The University of Queensland, Brisbane, Australia — [3]James Cook University, Cairns, Australia

The origin of photocurrent losses in the power-generating regime of organic solar cells (OSCs) remains a controversial topic, although recent literature suggests the importance of bimolecular recombination in determining the bias dependence of the photocurrent. Here we studied the steady-state recombination dynamics in OSCs with different hole mobilities from short-circuit to maximum power point (Adv. Energy Mater. DOI: 10.1002/aenm.201601379). We show that in this bias regime, first-order recombination outweighs bimolecular recombination of free charges. We demonstrate that the first-order losses increase with decreasing slower carrier mobility and attribute them to recombination of photogenerated and injected charges and/or geminate recombination. We also present how the competition between bimolecular recombination and extraction can be described using a simple figure of merit under consideration of space charge effects (J. Phys. Chem. Lett. DOI: 10.1021/acs.jpclett.6b02106). The experimental results obtained on 25 different OSCs represent a conclusive understanding of bimolecular recombination and allow to minimize these losses for given device parameters. Nevertheless, more work is necessary to understand the recombination losses in the power-generating regime in full generality.

CPP 41.6 Wed 16:30 ZEU 260

Experimental and simulated illumination dependent conductivity changes in organic bulk hetero junction solar cells — •Arne Müller, Vladislav Jovanov, and Veit Wagner — Jacobs University Bremen,Campus Ring 1, 28579 Bremen, Deutschland

The usage of organic solar cells for indoor application or for wearable electronics requires a good functionality for a wide range of irradiated light intensities. Therefore the IV behaviour of bulk hetero junction solar cells is analysed for a large variety of illumination intensities. We find that the IV-characteristic differs from the predictions of the Shockley-model, which is attributed to the low mobility of the charge carriers. The results are compared to drift-diffusion device simulations and with a simplified device model based on the Fermi-level spitting behaviour inside the semiconductor. In addition JscVoc experiments were performed to gain an insight into the series-resistance properties at different light intensities. As expected we found that the conductivity of the device is changed due to the light created charge carriers. The findings of the JscVoc analysis are then compared to our improved device model.

15 min break

CPP 41.7 Wed 17:00 ZEU 260

Design and Application of NIR Absorbing Donator Materials for Efficient Organic Solar Cells — •Sebastian Schellhammer[1,2,3], Frank Ortmann[1,2], and Gianaurelio Cuniberti[1,2,3] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden — [2]Dresden Center for Computational Materials Science, TU Dresden — [3]Center for Advancing Electronics Dresden, TU Dresden

Recently, fluorene-functionalized aza-BODIPYs have been successfully applied as donor material in organic solar cells.[1] Optimized bulk heterojunction solar cells with C60 have yield power conversion efficiencies up to 4.5 %, rendering the compounds highly competitive among other NIR-absorbing small-molecule donor materials. Based on an analysis of electronic properties, internal reorganization energies, and the optical properties of more than 100 aza-BODIPYs we give guidelines for the design of further optimized materials for solar cell applications. The observed independence of most of the functionalization strategies makes them an ideal material class for tailor-made donor materials that can cover a broad range of absorption, charge transport, and energetic regimes.

[1] M. Lorenz-Rothe, K. S. Schellhammer et al. Adv. Electron. Mater. 2, 1600152 (2016).

CPP 41.8 Wed 17:15 ZEU 260

Manipulating the morphology in printed organic solar cells — •Stephan Pröller[1], Daniel Moseguí Gonzáles[2], Chenhui Zhu[3], Alexander Hexemer[3], Peter Müller-Buschbaum[2], and Eva M. Herzig[1] — [1]TU München, Munich School of Engineering, Herzig Group, 85748 Garching, Germany — [2]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [3]Lawrence Berkeley National Laboratory, Advanced Light Source, Berkeley, USA

The nanomorphology can strongly influence the physical properties of organic thin films. For example, polymer:fullerene blends used in organic photovoltaics vary significantly in performance depending on the inner film morphology. To allow large-scale production of these devices, control of the nanostructure during the processing of the active layer is important. This firstly needs an understanding of the processes involved during the drying of the film. Using an industrial slot-die coater implemented into a synchrotron beamline we have successfully characterized the solidification process of an active layer using grazing incidence small and wide angle X-ray scattering (GISAXS/GIWAXS). We use the gained knowledge to further manipulate the structure of printed organic thin films by external intervention while printing. With this manipulation, we are able to positively influence the morphological evolution and thus the performance of the produced devices.

CPP 41.9 Wed 17:30 ZEU 260

On the Role of Triplet Excitons in Organic Solar Cells — •Andreas Sperlich[1], Stefan Väth[1], Hannes Kraus[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg

A strategy for increasing the conversion efficiency of organic photovoltaics has been to increase V_{OC} by tuning the energy levels of donor and acceptor components. However, this opens up a new loss pathway from an interfacial charge transfer state (CTS) to a donor triplet exciton (TE) state called electron back transfer (EBT), which is detrimental to device performance. To test this hypothesis, we study triplet formation in high performing blends of the fullerene $PC_{70}BM$ with either the polymer PTB7 [1] or the soluble small molecule p-DTS$(FBTTh_2)_2$ [2] and determine the impact of the morphology-optimizing additive 1,8-diiodoctane (DIO). Using photoluminescence and spin-sensitive optically and electrically detected magnetic resonance (ODMR, EDMR) measurements we find that TE formation does not only depend on the materials' energetics, but also on temperature and nano-morphology. Furthermore, we observe TEs in real devices under realistic working conditions even for the most efficient solar cells, which has implications not only for efficiency, but also for devices stability.

[1] H. Kraus, et al., Sci. Reps. 6, 29158 (2016)

[2] S. Väth, et al., Adv. Energy Mater., doi: 10.1002/aenm.201602016 (2016)

CPP 41.10 Wed 17:45 ZEU 260

Watching Paint Dry: The Impact of Diiodooctane on the Kinetics of Aggregate Formation in Thin Films of Poly(3-hexylthiophene) — •Markus Reichenberger[1], Sebastian Baderschneider[2], Daniel Kroh[1], Steffen Grauf[1], Juergen Koehler[2,3], Richard Hildner[2], and Anna Koehler[1,3] — [1]Experimental Physics II, University of Bayreuth, 95440 Bayreuth, Germany — [2]Experimental Physics IV, University of Bayreuth, 95440 Bayreuth, Germany — [3]Bayreuth Institute of Macromolecular Research (BIMF), University of Bayreuth, 95440 Bayreuth, Germany

We have investigated how the addition of 1,8-diiodooctane (DIO) alters the formation of disordered and ordered phases in a film of poly(3-hexylthiophene-2,5-diyl) (P3HT). By combining in situ time-resolved absorption spectroscopy with 60 ms time resolution, optical and transmission electron microscopy and spatially resolved photoluminescence spectroscopy, we show that, in addition to the excitonic coupling, the film formation process during spin-coating as well as the subsequent long-time film drying process differ significantly when DIO is added to a solution of P3HT. During spin-coating, the addition of DIO reduces the actual time for transformation from disordered to ordered phase, even though it increases the time until the disorder-order transition sets in. In place of a solidification front, we observe an all-over solidification throughout the entire film. The phase separation between nonaggregated and aggregated phase increases when using DIO, with compositional variation in the content of aggregated phase on a micrometer scale.

CPP 41.11 Wed 18:00 ZEU 260

Bicontinuous Morphologies in Ternary Blends of Molecular Glasses — •Michael Grimann, Evgeny Tatarov, and Thomas Fuhrmann-Lieker — University of Kassel, Institute of Chemistry and Center for Interdisciplinary Nanostructure Science and Technology, 34109 Kassel, Germany

We demonstrate nanoscale phase separated morphologies in organic functional materials. These glassy compounds comprise structural motifs known from OLED or organic laser materials like oligophenyls and triarylamines as electron donors. We developed electron acceptors containing perfluorinated aromatic moieties which lead to a miscibility gap with the respective donors. Binary blends thereof undergo phase separation via spinodal decomposition in equichoric compositions. Kinetics of this demixing process can be significantly slowed by addition of especially designed surfactant-like bipolar materials. The resulting bicontinuous morphologies of tuneable scale are useful for future random lasing and photovoltaic applications.

CPP 41.12 Wed 18:15 ZEU 260

Controlling the aggregation of native polythiophene during in situ polymerization — •Jenny Lebert, Eva M. Kratzer, Mihael Coric, Salma Mansi, and Eva M. Herzig — TU München, Munich School of Engineering, Herzig Group, 85748 Garching, Germany

Native polythiophene belongs to the class of conjugated, semiconducting polymers which become conductive upon doping and therefore offer a broad range of potential applications in organic electronics. While polythiophene itself is insoluble, it is possible to obtain solution processed thin films by employing an in situ polymerization technique. This way, the soluble monomers are deposited to the substrate and chemically linked afterwards. Since it is well known, that the performance of polymeric electronic devices depends strongly on the molecular interactions within the thin films, understanding and controlling the crystallization and film morphology are of crucial importance.

Here, we would like to present the possibilities of influencing the aggregation of the polythiophene chains in the film formation process by varying easily changeable synthetic parameters. The synthesized polymer films are analyzed regarding their optic and electronic properties as well as their morphology to show a clear dependence of the chosen synthetic path on the final film characteristics.

CPP 42: Charged Soft Matter, Ionic Liquids and Polyions I

Time: Wednesday 15:00–18:00 Location: ZEU 114

CPP 42.1 Wed 15:00 ZEU 114

Reactivity and structure of NaOH solutions from neural-network-based simulations — •Matti Hellström and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Germany

Sodium hydroxide (NaOH) is soluble in water up to very high concentrations and has many applications in chemical industry. Using a high-dimensional neural network potential for NaOH(aq) based on dispersion-corrected DFT calculations, we have performed large-scale molecular dynamics simulations with close to ab initio quality. The simulations reveal an unexpected multitude of concentration-dependent presolvation mechanisms governing the proton-transfer rate from H_2O to OH^- [1], and a large variety of coordination environments around the Na^+ ions [2].

[1] M. Hellström, J. Behler. *J. Phys. Chem. Lett.* **7** (2016) 3302

[2] M. Hellström, J. Behler. *Phys. Chem. Chem. Phys.* DOI: 10.1039/C6CP06547C

CPP 42.2 Wed 15:15 ZEU 114

Preferential solvation and ion association properties in aqueous dimethyl sulfoxide solutions — •Anand Narayanan Krishnamoorthy, Johannes Zeman, Christian Holm, and Jens Smiatek — Institute for Computational Physics - University of Stuttgart

We study the solvation and the association properties of ion pairs in aqueous dimethyl sulfoxide (DMSO) solution by atomistic molecular dynamics (MD) simulations. The ion pair is composed of two lithium and a single sulfonated diphenyl sulfone ion whose properties are studied under the influence of different DMSO concentrations. For increasing mole fractions of DMSO, we observe a non-ideal behavior of the solution as indicated by the derivatives of the chemical activity. Our findings are complemented by dielectric spectra, which also verify a complex DMSO-water mixing behavior. In agreement with these results, further simulation outcomes reveal an aqueous homoselective solvation of the ion species which fosters the occurrence of pronounced ion association constants at higher DMSO mole fractions. The consequences of this finding are demonstrated by lower ionic conductivities for increasing concentrations of DMSO.

CPP 42.3 Wed 15:30 ZEU 114

Image-charge effects on the dissociation of acids at dielectric discontinuities — •Philip Loche, Alexander Schlaich, Cihan Ayaz, Senta Volkenandts, and Roland Netz — Department of Physics, Free University Berlin, Arnimallee 14, 14195 Berlin, Germany

In colloid and interface sciences image-charge effects are considered to play a key role for ion transport and double layer attraction. Image-charge effects are also an important component for the self-energy of ions or functional groups and thus contribute to the dissociation constant of acids.

We use molecular dynamics simulations in combination with the local dielectric permittivity tensor and the solution of the tensorial Green's functions to investigate electrostatic effects at interfaces. The potential of mean force and free energy calculations are deployed for simple ions and functional groups. The analytical self-energy obtained from the tensorial Green's function is compared to simulation results.

CPP 42.4 Wed 15:45 ZEU 114

Cation-induced hydration effects cause lower critical solution temperature behavior in protein solutions — •Olga Matsarskaia[1], Michal K. Braun[1], Felix Roosen-Runge[2], Marcell Wolf[1], Fajun Zhang[1], Roland Roth[3], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]Institut Laue-Langevin, Grenoble, France — [3]Institut für Theoretische Physik, Universität Tübingen

Systems consisting of negatively charged proteins and trivalent salts feature strong short-range attractive forces and exhibit a rich phase behaviour including reentrant condensation, clustering and crystallisation [1]. Here, we report a *lower critical solution temperature* liquid-liquid phase separation (LCST-LLPS) behaviour in a system of bovine serum albumin (BSA) and the trivalent salt YCl_3. Combining isothermal titration calorimetry (ITC) and ζ potential data into a comprehensive model, we show that cation-protein binding is an endothermic and thus entropy-driven process. We attribute the entropic contribution to a partial release of hydration water molecules around Y^{3+} cations and protein carboxyl groups. Our findings have implications for the general understanding of hydration-mediated interactions of soft matter.

[1] Zhang *et al.* Pure & Appl. Chem. 2014, 86, 191-202; [2] Matsarskaia *et al.* JPCB 2016, 120, 7731-7736.

Invited Talk CPP 42.5 Wed 16:00 ZEU 114

Aqueous Ionic Liquids and Their Influence on Peptide Conformations: Denaturation and Dehydration Mechanisms — •Jens Smiatek — Institut für Coputerphysik, Universität Stuttgart, D-70569 Stuttgart, Germany

The influence of low concentrated aqueous ionic liquid (ILs) solutions on protein structures has attracted a lot of interest in the last years. This can be mostly attributed to the distinct roles of the aqueous ILs as protein protectants or protein denaturants. I will review the results of atomistic molecular dynamics (MD) simulations to study the influence of different ILs on the conformational properties of a short hairpin peptide. The results reveal distinct binding and denaturation effects for 1-ethyl-3-methylimidazolium (EMIM) in combination with the different anions chloride (CL), tetrafluoroborate (BF4) and acetate (ACE). The simulation outcomes indicate that ILs with larger anions induce a stronger dehydration effect which is accomplished by a more pronounced accumulation behavior of the individual ion species around the peptide. All findings can be related to the implications of the Kirkwood-Buff theory, which provides a thermodynamic explanation for the denaturation strength in terms of the IL accumulation behavior. The outcomes of this analysis are in good agreement with the results of metadynamics simulations to determine the energetically most favorable conformations of the peptide in presence of the individual aqueous ILs. All findings indicate that the denaturation strength decreases in the order EMIM/ACE, EMIM/BF4 and EMIM/CL, which coincides with the size of the anion species.

15 min break

CPP 42.6 Wed 16:45 ZEU 114

Dynamics of Room Temperature Ionic Liquids: A ^{1}H and ^{19}F NMR Relaxometry and Diffusiometry study — •Manuel Becher and Michael Vogel — TU Darmstadt Solid State Physics, Darmstadt, Germany

Room Temperature Ionic Liquids (RTIL) are salts with a low melting point and vapour pressure, caused by a rather big and asymmetric cation. They are usually glass forming systems with complex and heterogeneous molecular dynamics. The combination of different cations and anions opens wide ranges of chemical and physical applications, e.g. as solvents or fluid electrolytes, and their optimization. Hence, a fundamental understanding of molecular dynamics is of crucial importance. Here, imidazolium based RTILs with an $[Tf2N]^-$ anion are in the experimental focus, with a variation of alkyl chain lengths at the cation so as to vary structural and dynamical heterogeneity. Nuclear Magnetic Resonance (NMR) provides access to glassy dynamics in wide range of temperature and length scales. Due to its isotope sensitivity the dynamical behaviour of different molecules/molecular groups can be separated. In a static field gradient, we measure the self-diffusion coefficient of the cation (^{1}H) and anion (^{19}F), revealing hints to clustering. Field-Cycling relaxometry provides frequency-dependent relaxation times $T_1(\omega)$ and yields translational and rotational correlation times as well as insight into local dynamics. Comparing long-range self-diffusion with short-range structural relaxation, we analyze cation-anion couplings against the background of alkyl-chain length dependent structural heterogeneities.

CPP 42.7 Wed 17:00 ZEU 114

A Coarse-Grained Model for Polyionic Liquids — •Alexander Weyman[1], Jens Smiatek[1], Markus Bier[2], and Christian Holm[1] — [1]Institut for Computational Physics, University of Stuttgart — [2]Max Planck Institute for Intelligent Systems

Polyionic liquids or polymerized ionic liquids (PILs) are a relatively new class of polyelectrolytes that combine both the advantages of polymeric materials and the unique properties of ionic liquids and therefore have become the focus of scientific interest in recent years.

We show results from molecular dynamics (MD) simulation using a coarse-grained model for polyionic liquids in order to analyze structural features and transport properties. The polymer chains are described by a bead-spring model where the single PIL monomers are represented by single beads that are interconnected via bond potentials.

Following the observation of microphase separation in dense bulk systems of ionic liquids, dense systems of polyionic liquids are simulated, and partial structure factors are calculated for the quantitative analysis of the likewise occurring microphases.

Using a classical density functional theory framework, a selection of partial structure factors is calculated and compared with MD simulations.

Furthermore, we also find an enhancement of the conductivity, if the PILs are confined between two plane-parallel interfaces, due to the occurrence of a larger conductivity near the interfaces which is in agreement with experimental findings that have speculated about the occurrence of conductivity channels.

CPP 42.8 Wed 17:15 ZEU 114

Dielectric study on mixtures of ionic liquids — •Pit Sippel[1], Erik Thoms[1], Daniel Reuter[1], Alois Loidl[1,2], and Stephan Krohns[1,2] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany — [2]Institute for Materials Resource Management, University of Augsburg, 86152 Augsburg, Germany

Ionic liquids are salts that are liquid below 100 °C and offer outstanding properties (e.g., low volatility and high electrochemical stability). These make them promising candidates for solvent-free electrolytes to improve energy storage systems [1]. However, most ionic liquids exhibit low conductivity, hampering their applicability in supercapacitors and battery systems. We demonstrate the tuning of the conductivity via mixing various ionic liquids. An increased conductivity has been reported for particular mixing series. Nonetheless, these are exceptions and most mixing series behave close to linear mixing-laws. To gain more insight into the molecular dynamics we performed detailed investigations by dielectric spectroscopy and differential scanning calorimetry on two mixing series of ionic liquids. The analysis of the glass temperatures and the thorough evaluations of the measured dielectric spectra reveal that the dynamics in these mixtures are well defined by the fractions of their parent compounds. Moreover the room-temperature conductivity in these mixtures is still directly related to their glass properties, as in pure ionic liquids [2].

[1] D. R. MacFarlane, *et al.*, Energy Environ. Sci. **7,** 232 (2014).

[2] P. Sippel *et al.*, Sci. Rep. **5,** 13922 (2015).

CPP 42.9 Wed 17:30 ZEU 114

Insights on the diversity of smectic phases in ionic liquid crystals — •Hendrik Bartsch[1,2], Markus Bier[1,2], and Siegfried

Dietrich[1,2] — [1]Max Planck Institute for Intelligent Systems, 70569 Stuttgart, Germany — [2]Institute of Theoretical Physics IV, University of Stuttgart, 70569 Stuttgart, Germany

Ionic liquid crystals (ILCs) can be described as anisotropic molecules, which carry charges and therefore combine properties of liquid crystals, e.g. mesophases, and ionic fluids, e.g. low melting temperatures and tiny triple-point pressures. However, the combination of both, orientational degrees of freedom and electrostatics renders a particular challenge for theoretical studies.

Recently a promising model of ILCs has been proposed and studied within the framework of density functional theory [1]. It turns out, that the phase diagram is strongly affected by the molecules' properties, i.e. the length-to-breath ratio, the position of charges and the interaction strengths. Here, we report on very recent findings on the phase behavior of ILCs obtained by means of density functional theory and Monte Carlo simulations. The most striking is the occurrence of a novel, second smectic A phase at low temperature, whose layer spacing is larger than that of the ordinary high-temperature smectic A phase and increasing upon decreasing temperature at constant packing fraction or pressure.

[1] S. Kondrat, M. Bier, and L. Harnau, J. Chem. Phys. **132**, 184901 (2010)

CPP 42.10 Wed 17:45 ZEU 114

Determination of the optical constants of ionic liquids by ellipsometry — •Xia Wu[1], Maren Muntzeck[2], Teresa de los Arcos[3], Ignacio Giner[3], Guido Grundmeier[3], René Wilhelm[2], and Thorsten Wagner[1] — [1]Inorganic and analytical chemistry, Department of Chemistry, University of Paderborn, Warburger Straße 100, D-33098, Paderborn, Germany — [2]Organic chemistry, Department of Chemistry, University of Paderborn, Warburger Straße 100, D-33098, Paderborn, Germany — [3]Technical chemistry, Department of Chemistry, University of Paderborn, Warburger Straße 100, D-33098, Paderborn, Germany

We determined the optical constants (complex refractive index, dispersion and temperature coefficient) of ionic liquids by ellipsometry method mainly in visible range (360 nm - 1000 nm). We focus on the ionic liquids with high refractive indices (n > 1.7) since it is not possible to measure this high index by normal refractometer. We synthesized ionic liquids with such high indices. These high index ionic liquids can be used as index matching liquids in determination of refractive indices of metal oxides inside photonic crystals or porous materials in general. These ionic liquids are particularly suitable for index matching, because they are stable (low vapor pressure) and less toxic than commercial available index matching liquids with equally high indices [1].

Reference: [1] M. Deetlefs, K. R. Seddon, M. Shara, New Journal of Chemistry 30, 317-326 (2006); doi: 10.1039/b513451j

CPP 43: Fluids and Glasses II

Time: Wednesday 15:00–16:00 Location: ZEU 255

CPP 43.1 Wed 15:00 ZEU 255

Chemical Potential Calculation of Dense Fluids using Hamiltonian Adaptive Resolution Simulation — •Maziar Heidari, Robinson Cortes-Huerto, Kurt Kremer, and Raffaello Potestio — Max Planck Institute for Polymer Research, Mainz, Germany

The calculation of chemical potential of fluids is a relevant and challenging problem in computational chemistry and physics. Here, we propose a method which employs the recently multi-scale Hamiltonian Adaptive Resolution Simulation (H-AdResS) method to calculate the chemical potential of dense fluids. In H-AdResS, the simulation domain is subdivided in regions of high and low resolutions, coupled through a hybrid region. Since the dynamics of particles are obtained from a global Hamiltonian, the generated statistical ensembles of the system are well-defined. In our method, the fluid within the high resolution region is coupled with an ideal gas of non-interacting particles, and to enforce a uniform density profile an external force is computed on-the-fly and applied. Then the converged compensation forces are integrated across the hybrid region to obtain the Gibbs free energy difference between the two resolutions. The resulting Gibbs free energy is related to the excess chemical potential of the fluid with respect to the ideal gas. We validated this method by calculating the excess chemical potentials of fluid mixtures.

CPP 43.2 Wed 15:15 ZEU 255

A Refined Polarizable Water Model for the Coarse-Grained MARTINI Force Field — •Julian Michalowsky[1], Lars Schäfer[2], Johannes Zeman[1], Christian Holm[1], and Jens Smiatek[1] — [1]Institute for Computational Physics, University of Stuttgart, Allmandring 3, D-70569 Stuttgart, Germany — [2]Center for Theoretical Chemistry, Faculty of Chemistry and Biochemistry, Ruhr-University, Universitätsstraße 150, D-44780 Bochum, Germany

We propose a refined version of the polarizable MARTINI water model designed for the use with long-range electrostatics. Our new model improves the resemblance of the experimentally measured water mass density at room temperature and matches the experimentally measured dielectric constant of water. Our investigations show that the new model performs stably with a variety of commonly used sets of simulation parameters, remaining fully applicable within a reaction field framework. The oil/water partitioning behavior of uncharged MARTINI beads is thoroughly investigated: Lennard-Jones interactions between our new model and the remaining MARTINI beads are tuned to reproduce the hydration free energies obtained with the original polarizable water model. The cross-interactions with charged bead types are matched to the experimentally observed area per lipid of a solvated dipalmitoylphosphatidylcholine (DPPC) lipid bilayer. We additionally analyzed the potentials of mean force between different sample pairs solvated in the refined polarizable water model and compared the results to reference data obtained using the original water model and atomistic approaches.

CPP 43.3 Wed 15:30 ZEU 255

Diverging time scale in the dimensional crossover for liquids in strong confinement — •Suvendu Mandal and Thomas Franosch — Institut für Theoretische Physik, Leopold-Franzens-Universität Innsbruck, Technikerstr. 21A, A-6020 Innsbruck, Austria

We study a strongly interacting dense hard-sphere system confined between two parallel plates by event-driven molecular dynamics simulations to address the fundamental question of the nature of the 3D to 2D crossover. As the fluid becomes more and more confined the dynamics of the transverse and lateral degrees of freedom decouple, which is accompanied by a diverging time scale separating 2D from 3D behavior. Relying on the time-correlation function of the transversal kinetic energy the scaling behavior and its density-dependence is explored. Surprisingly, our simulations reveal that its time-dependence becomes purely exponential such that memory effects can be ignored. We rationalize our findings quantitatively in terms of an analytic theory which becomes exact in the limit of strong confinement.

CPP 43.4 Wed 15:45 ZEU 255

Structure, Dynamics and Phase Behavior of a Discotic Liquid Crystal Confined in Nanoporous Anodic Aluminum Oxide Membranes — •Arda Yildirim[1], Kathrin Sentker[2], Patrick Huber[2], and Andreas Schönhals[1] — [1]Bundesanstalt für Materialforschung und -prüfung [BAM] — [2]Institut für Werkstoffphysik und -technologie, Technische Universität Hamburg-Harburg (TUHH)

Discotic liquid crystals (DLCs) are a promising class of soft matter for electronic applications. This is due to their ability to organize and stack themselves into columns in a hexagonal columnar mesophase, driven by the overlapping of the π-orbitals of their aromatic core. This leads to a high charge-carrier mobility along the column axis. Previous studies on DLCs showed that their properties, such as phase transition temperatures and enthalpies, are susceptible to nanoconfinement [1,2]. In this study, 2,3,6,7,10,11 hexakis[hexyloxy] triphenylene (HAT6), a triphenylene based DLC, was confined into parallel aligned cylindrical nanopores of anodic aluminum oxide (AAO) membranes by melt infiltration in the isotropic phase under an argon atmosphere. Furthermore, the pore surfaces of a series of membranes were chemically modified, resulting in a more hydrophobic pore surface than the unmodified ones. The structure, dynamics, and the phase behavior of HAT6 confined into modified and unmodfied nanopores of AAO were investigated by broadband dielectric spectroscopy and differential scanning calorimetry. Results will be discussed in detail.

[1] C. Krause and A. Schönhals, J. Phys. Chem. C, 2013, 117, 19712.

[2] C. Krause et al., Colloid Polym. Sci., 2014, 292, 1949.

CPP 44: Aktive Matter I (joint session DY/BP/CPP, organized by DY)

Time: Wednesday 15:00–19:00 Location: HÜL 186

CPP 44.1 Wed 15:00 HÜL 186

Flocking ferromagnetic particles — •Andreas Kaiser, Alexey Snezhko, and Igor S. Aranson — Materials Science Division, Argonne National Laboratory, 9700 South Cass Ave, Argonne, Illinois 60439, USA

Suspensions of microswimmers, show fascinating collective behaviours like clustering, flocking and turbulence [1]. Here, we demonstrate the discovery of ferromagnetic flocking colloids. The self-propulsion is an outcome of the spontaneous rotation of a ferromagnetic colloidal sphere in a vertical alternating (AC) magnetic field [2]. Depending on the frequency of this magnetic field, a sequence of transitions can be observed: from gas-like motion of individual particles to the onset of flocking and global rotation followed by a reentrant flocking and gas-like state for increasing frequency [3]. We also emphasize a subtle role of rotational noise: While the low-frequency flocking appears to be noise-insensitive, the reentrant flocking happens to be noise-activated. Moreover, we uncover a new relation between collective motion and synchronisation.

[1] T. Vicsek, A. Zafeiris, Physics Reports 517, 71 (2012)

[2] G. Kokot, D. Piet, G.M. Whitesides, I.S. Aranson, A. Snezkho, Scientific Reports 5, 9528 (2015)

[3] A. Kaiser, A. Snezkho, I.S. Aranson, Science Advances (submitted)

CPP 44.2 Wed 15:15 HÜL 186

Unexpected enhancement of rotational dynamics of self-propelled particles in a colloidal glass — •CELIA LOZANO[1,2], JUAN RUBEN GOMEZ-SOLANO[1], 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

It has been recently demonstrated that the glass transition of dense colloidal suspensions is progressively shifted by increasing activity of embedded self-propelled particles (SPP) [1]. However, it is not clear yet how the dynamics of such SPP becomes affected by the surrounding glassy environment. We experimentally investigate the active motion of spherical Janus particles within a cage created by a binary mixture of colloidal particles. We observe a dramatic enhancement of the rotational diffusion of active particles with increasing particle velocity and the density, in a similar fashion as SPP in semi-dilute polymer solutions [2]. This experimental approach allows us to measure, in parallel, the temporal evolution of the active particle and the passive colloidal suspension. Our findings suggest that these effects originate from the coupling between the thermal fluctuations of the particle and the surrounding heterogeneities, which displays large relaxation times of several seconds.

[1] Ni, R., Stuart, M. A. C. & Dijkstra, M. Nature communications 4, 2704 (2013). [2] Gomez-Solano, J. R., Blokhuis, A. & Bechinger, C. Phys. Rev. Lett. 116, 138301 (2016).

CPP 44.3 Wed 15:30 HÜL 186

Motility-Induced Phase-Separation of Microswimmers: Hydrodynamics and Phase-Equilibria — •Johannes Blaschke and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Hardenberg Str. 36, 10623 Berlin, Germany

Active motion of microorganisms and artificial microswimmers is relevant both to real world applications as well as for posing fundamental questions in non-equilibrium statistical physics. Microswimmers are often modelled as active Brownian particles, neglecting hydrodynamic interactions between them. However, real microswimmers, such as ciliated microorganisms, catalytic Janus particles, or active emulsion droplets, employ propulsion mechanisms reliant on hydrodynamics. Therefore, we use multi-particle collision dynamics to explore the influence of hydrodynamics on the collective behavior of spherical microswimmers in quasi-two-dimensional geometry [1].

A striking feature of the collective motion of microswimmers is that for sufficiently strong self-propulsion they phase-separate into dense clusters coexisting with a low-density gas phase. Here we examine the influence of hydrodynamic interactions on this motility-induced phase separation. The most striking difference with the phase diagram of active Brownian particles is that a larger mean density results in a lower density of the coexisting dilute phase, which is a clear signature of hydrodynamics. Furthermore, we find that pushers or pullers suppress phase separation by increasing the critical Péclet number.

[1] J. Blaschke, M. Maurer, K. Menon, A. Zöttl, and H. Stark, *Soft Matter* (2016), DOI:10.1039/C6SM02042A.

CPP 44.4 Wed 15:45 HÜL 186

Synthetic Janus microswimmers moving under confinement in viscoelastic media — •Juan Ruben Gomez Solano[1], Mahsa Sahebdivani[1], and Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universitaet Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Max-Planck-Institut fuer Intelligente Systeme, Heisenbergstrasse 3, 70569 Stuttgart, Germany

The motion of many natural microswimmers, e.g. bacteria and spermatozoa, commonly takes place in viscoelastic media and under confinement close to solid walls. Recent experiments demonstrate that active colloids in Newtonian liquids can be hydrodynamically and phoretically trapped or guided by solid walls depending on the surrounding flow field and on the geometry of the confinement [1-3]. In our work, using spherical Janus microswimmers activated by light in a semidilute polymer solution [4], we experimentally investigate how viscoelasticity affects the motion of such self-propelled particles when approaching or leaving a flat wall. Unlike self-propulsion in Newtonian fluids, we find a strong particle-wall repulsion induced by the surrounding viscoelastic liquid over large distances from the wall. We show that this phenomenon has dramatic consequences for the particle translational and rotational dynamics in more complex confined geometries, as well as for collective motion in crowded environments.

[1] G. Volpe et al., Soft Matter 7, 8810 (2011). [2] D. Takagi et al., Soft Matter 10, 1784 (2014). [3] J. Simmchen, Nat. Comm. 7, 10598 (2016). [4] J. R. Gomez-Solano, A. Blokhuis, and C. Bechinger, Phys. Rev. Lett. 116, 138301 (2016).

CPP 44.5 Wed 16:00 HÜL 186

Dynamics of microswimmer molecules — Sonja Babel, Niklas Küchler, Hartmut Löwen, and •Andreas M. Menzel — Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany

In recent years, the dynamical properties of individual microswimmers have been investigated intensively. The same applies for their collective dynamical behavior in dilute and dense suspensions. Here we address an intermediate level. We study the dynamics of compound objects of coupled swimmers that we term “microswimmer molecules” [1,2].

First, we address three spherical magnetic microswimmers connected by elastic springs to a straight object [1]. The magnetic interactions support the straight arrangement. However, with increasing active drive, hydrodynamic interactions destabilize the straight shape. Technically, this occurs via a subcritical Hopf bifurcation. The oscillatory feature of this bifurcation is connected to a cork-screw-like motion of the molecule.

Second, we consider an active microswimmer coupled by elastic springs to one or more passive swimmers [2]. The dynamics of this type of molecule in an external planar swirl flow is investigated, while hydrodynamic interactions are neglected to lowest order. Because of the finite extension and deformability of these molecules, interesting dynamical features arise. They comprise an expulsion from or undertow into the swirl, rotations of the deformed trajectories, and changes in the sense of the trajectory rotations.

[1] Babel et al., *EPL (Europhys. Lett.)* **113**, 58003 (2016).

[2] Küchler et al., *Phys. Rev. E* **93**, 022610 (2016).

CPP 44.6 Wed 16:15 HÜL 186

Microscopic derivation of the hydrodynamics of active-

Brownian-particle suspensions — Stefano Steffenoni[1], •Gianmaria Falasco[2], and Klaus Kroy[2] — [1]Max planck for the mathematics in the science, leipzig — [2]Institute for theoretical physics, leipzig

We derive the hydrodynamic equations of motion for a fluid of active particles described by under- damped Langevin equations that reduce to the Active-Brownian-Particle model, in the overdamped limit. The contraction into the hydrodynamic description is performed by locally averaging the particle dynamics with the non-equilibrium many-particle probability density, whose formal expres- sion is found in the physically relevant limit of high-friction through a multiple-time-scale analysis. This approach permits to identify the conditions under which self-propulsion can be subsumed into the fluid stress tensor and thus to define systematically and unambiguously the local pressure and surface tension of the active fluid.

15 min. break

CPP 44.7 Wed 16:45 HÜL 186

Determination of the phase behavior and the critical point in systems of active particles in depletants — •Jonathan Tammo Siebert[1], Benjamin Trefz[1,2], Thomas Speck[1], Kurt Binder[1], and Peter Virnau[1] — [1]Department of Physics, Johannes Gutenberg University of Mainz, D-55128 Mainz, Germany — [2]Graduate School Materials Science in Mainz, D-55128 Mainz, Germany

We study a modified, active variant of the well-known Asakura-Oosawa model for colloid-polymer mixtures. Activity is introduced as Vicsek-like self-propulsion. This system already undergoes phase separation in case of zero propulsion. In the driven case, the binodal lines are shifted towards lower densities.

Building on earlier results for the binodal line, we completed the phase diagram by determination of the critical point, using a subsystem-block-density distribution analysis. In addition to understanding critical phenomena in this specific system far from equilibrium, the proposed method can serve as a recipe to find critical points and the associated exponents for other types of active particles.

CPP 44.8 Wed 17:00 HÜL 186

Clustering of nematic active particles in low Reynolds number Navier-Stokes flow — •Rebekka Breier, Cristian C. Lalescu, Devin Waas, Michael Wilczek, and Marco G. Mazza — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen

Large groups of self-propelled particles are ubiquitous in nature, from flocks of starlings and herds of wildebeests down to schools of fish and groups of bacteria or algae. Many of these creatures exist in (possibly mildly) turbulent habitats, like motile plankton in the pycnocline of the ocean. We study large systems of self-propelled, nematically aligning, hard core particles by means of molecular dynamic simulations which inhabit a turbulent environment. We investigate the active dynamics and compare the results from kinematic simulations ("synthetic turbulence") with direct numerical simulations of the turbulent background field. We find a "sweet spot" for clustering, that is, an optimal strength of turbulence leads to very dense small-scale clusters. We explain the mechanism that induces clustering. Moreover, we investigate the effect of hard cores compared to point particles, and also give the appropriate dimensionless numbers to describe the dynamic transitions.

CPP 44.9 Wed 17:15 HÜL 186

Reinforcement learning of artificial microswimmers — •Santiago Muiños-Landin[1], Keyan Ghazi-Zahedi[2], and Frank Cichos[1] — [1]Molecular Nanophotonics. University of Leipzig. Institut for Experimental Physics I — [2]Information Theory of Cognitive Systems, Max Planck Institute for Mathematics in the Sciences

Reinforcement Learning (RL) is a special area of the Machine Learning discipline which consist in the search of an optimal policy in the context of Markovian Decision Processes (MDP). Learning is based on the interaction of the system with its environment and is guided by sparse rewards. In RL a policy is a function that connects the available actions that an agent can execute with the states where this agent can be located at. MDPs were already proposed as a model for the navigation of natural microswimmers. Here we present now a method that uses this RL in order to achieve an autonomous explorative behavior from a self-thermophoretic microswimmer. We implement it experimentally by photon nudging to reach reinforcement learning of a symmetric microswimmer.

CPP 44.10 Wed 17:30 HÜL 186

Self-propelled motion of an extra particle in a two-dimensional plasma crystal — •Ingo Laut, Christoph Räth, Sergey K. Zhdanov, Volodymyr Nosenko, Gregor E. Morfill, and Hubertus M. Thomas — Deutsches Zentrum für Luft- und Raumfahrt, Forschungsgruppe Komplexe Plasmen, 82234 Weßling, Germany

Plasma crystals consist of charged microparticles that levitate in a weakly ionized gas. In these nonequilibrium systems the particle interaction is nonreciprocal due to flowing ions. Plasma crystals were successfully used to study dynamical effects in liquids and solids at the kinetic level and have the potential to also enable the study of active particles.

Here, we analyze in simulations and theory the self-propelled motion of an "extra" particle in a two-dimensional plasma crystal. Experimental observations [1] showed that the extra particle is confined in a channel of two neighboring rows of particles and moves persistently through the crystal. We use the simple model of a pointlike ion wake charge to reproduce this intriguing effect in simulations. We show that the nonreciprocity of the particle interaction, owing to the plasma flow, is responsible for a broken symmetry of the channel that enables the self-propelled motion of the extra particle [2].

[1] C.-R. Du, V. Nosenko, S. Zhdanov, H. M. Thomas, and G. E. Morfill, Phys. Rev. E **89**, 021101(R) (2014)

[2] I. Laut, C. Räth, S. K. Zhdanov, V. Nosenko, G. E. Morfill, and H. M. Thomas, accepted for publication in Phys. Rev. Lett.

CPP 44.11 Wed 17:45 HÜL 186

Dynamics of model bacteria in dense polymer suspensions and networks — •Andreas Zöttl and Julia M Yeomans — Rudolf Peierls Centre for Theoretical Physics, University of Oxford, UK

Swimming bacteria, such as Helicobacter pylori, Pseudomonas aeruginosa and sperm cells, move through viscoelastic fluids, such as mucus, in vivo. Theoretical models for these complex fluids are typically based on continuum equations which assume a constant density of sufficiently small polymers, homogeneously embedded in a Newtonian fluid. However, real viscoelastic fluids are more structured when considered on the length scale of a microswimmer: they can consist of heterogeneously distributed, up to micrometer long, macromolecules such as mucin polymers.

Here we present results of coarse-grained hydrodynamic simulations of a flagellated bacterium swimming in explicitly modeled macromolecular polymer solutions and cross-linked networks. We find a remarkable increase in the bacterium's swimming speed at high polymer density. We further discuss the effect of polymer properties such as length, stiffness and cross-linking. We also report the flow fields and the local polymer properties in the vicinity of the bacterium, which can be strongly influenced by its motion.

CPP 44.12 Wed 18:00 HÜL 186

Rheology and shear-induced dynamics of passive and active anisotropic colloids — •Henning Reinken and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We investigate the rheology of passive and active fluids focusing on shear-induced instabilites and emerging spatiotemporal structures. Prominent examples of active matter, which is composed of self-driven units converting energy into motion on the microscopic scale, are anisotropic colloidal particles with polar or nematic interactions. Already in the passive case, these systems show very interesting rheological properties including oscillatory orientational states and shear banding [1]. Introducing activity into the system modifies the rheology and leads to additional instabilities [2].

We study the rheological properties via the Doi-Hess theory [1], a continuum theoretical approach. In this framework, the orientational order parameter is coupled to the flow via the stress tensor, which can be extended to include an active stress [2]. In particular, we focus on parameter regimes where interesting spatiotemporal structures like banded states or active turbulence [3] emerge and discuss the differences between active and passive systems.

[1] R. Lugo-Frías, H. Reinken, S. H. L. Klapp, Eur. Phys. J. E **39**: 88 (2016).

[2] M. C. Marchetti et al. Rev. Mod. Phys. **85**, 1143 (2013).

[3] S. Heidenreich, J. Dunkel, S. H. L. Klapp, M. Bär, Phys. Rev. E

94, 020601(R) (2016).

CPP 44.13 Wed 18:15 HÜL 186

Effective interactions of active particles: interfacial phase behavior and swim pressure — •René Wittmann, Abhinav Sharma, and Joseph Brader — Departement für Physik, Universität Fribourg, 1700 Fribourg, Schweiz

We employ classical density functional theory to study the self-organization in active systems. Using a first-principles approach, we map the self-propulsion onto an effective pair interaction potential, which has been shown [1] to account for the motility-induced phase separation (MIPS) observed for active Brownian particles. We further introduce an effective external potential and investigate inhomogeneous situations.

Solely as a result of their activity, we predict [2] that active (Brownian) particles undergo a variety of interfacial phase transitions, e.g., wetting and capillary condensation in purely repulsive systems or drying and capillary evaporation of attractive colloids. We explain why the effective thermodynamic pressure and interfacial tension do not coincide with the mechanical results, which we recover by embedding the presented effective-potential approach within a more general (dynamical) framework. Finally, we comment on situations with a non-vanishing particle current [3].

[1] T. F. F. Farage, P. Krinninger and J. M. Brader, Phys. Rev. E **91**, 042310 (2015).
[2] R. Wittmann and J. M. Brader, Europhys. Lett. **114**, 68004 (2016).
[3] A. Sharma, R. Wittmann, J. M. Brader, arXiv:1611.03897 (2016).

CPP 44.14 Wed 18:30 HÜL 186

Patterns in chemically interacting microswimmers: Do they really exist? — •Benno Liebchen[1], Davide Marenduzzo[1], and Michael E. Cates[2] — [1]SUPA, School of Physics and Astronomy, University of Edinburgh, Edinburgh EH9 3FD, United Kingdom — [2]DAMTP, Centre for Mathematical Sciences, University of Cambridge, Cambridge CB3 0WA, United Kingdom

Chemotaxis is the directed motion of particles in response to a gradient in a chemical signal. It allows micro-organisms, like bacteria, to find food and to escape from toxins. Some micro-organisms can produce the species to which they respond themselves and use chemotaxis for signalling. Remarkably, artificial Janus colloids that swim by catalysing reactions in a bath naturally feature chemical interactions and thereby provide a synthetic analogue to signalling micro-organisms. While, it is well known that cases where these interactions are attractive lead to clustering and phase separation, we have recently demonstrated that the purely repulsive case does not simply stabilize the uniform phase but creates a versatile new route to pattern formation in active systems.

In this talk, I will briefly review our work on chemorepulsive pattern formation and will focus the question on how generic and realistic these patterns are for Janus colloids. Our work unveils a fundamental link between autophoresis and chemotaxis leading to a massive collapse of parameter space and generic instability criteria which we confirm using particle based simulations.

CPP 44.15 Wed 18:45 HÜL 186

Kinetic theory of self-propelled particles: von Mises distribution and Chapman-Enskog expansion — •Rüdiger Kürsten and Thomas Ihle — Institut für Physik, Ernst-Moritz-Arndt Universität Greifswald

We consider Vicsek-type models [1] with multi-particle interactions and discrete time dynamics. Starting from the exact evolution equation for the N-particle probability distribution, an Enskog-like kinetic equation is derived. Recently, the von Mises distribution and an geometric series ansatz were proposed to treat this nonlinear integral equation [2,3]. We critically assess them for a Vicsek-model with bounded-confidence interactions. Both approaches recover the qualitative behavior of the system but the von Mises distribution causes large deviations in certain parameter regions [4]. We extend the von Mises approximation by an additional term that leads to much better agreement. The geometric series ansatz for the Fourier modes of the probability density is typically very accurate but fails for very weak noise. We therefore suggest an alternative approach – a Gaussian ansatz – for the higher modes, which is robust at all noises. Furthermore, we present a non-standard Chapman-Enskog expansion with a fast time scale. This expansion is used to derive the macroscopic transport equations from the microscopic collision rules. We discuss the expressions for the transport coefficients, which become simple in the limit of infinite density.

[1] Phys. Rev. Lett. 75 (1995) 1226 [2] J. Stat. Mech. (2015) P10017

[3] Phys. Rev. E 90 (2014) 063315 [4] arXiv:1611.00624

CPP 45: Biomaterials and Biopolymers (joint session BP/CPP, organized by BP)

Time: Wednesday 15:00–17:15 Location: SCH A251

CPP 45.1 Wed 15:00 SCH A251

The microstructural function of the tendon-bone insertion — •Leone Rossetti[1], Lara A. Kuntz[1,2], Elena Kunold[3], Jonathan Schock[1], Kei W. Müller[4], Heinrich Grabmayr[1], Josef Stolberg-Stolberg[5], Franz Pfeiffer[1], Stephan A. Sieber[3], Rainer Burgkart[2], and Andreas R. Bausch[1] — [1]Physik Department,TU München,D-85748 Garching, Germany — [2]Klinik für Orthopaedie und Sportorthopaedie, Klinikum rechts der Isar, TU München, D-81675 München, Germany — [3]CIPSM, Department of Chemistry, TU München, D-85747 Garching, Germany — [4]Institute for Computational Mechanics , TU München, D-85748 Garching, Germany — [5]University Hospital Münster, D-48149 Münster, Germany

The exceptional mechanical properties of the connection of tendon to bone rely on an intricate interplay of its biomolecular composition, microstructure and micromechanics. Here we identify that the Achilles tendon insertion is characterized by a stress reducing mechanism within an interfacial zone of 500 micrometres, with a distinct fiber organisation and biomolecular composition. Proteomic analysis detects enrichment in the interface region that are predominantly involved in cartilage and skeletal development as well as proteoglycan metabolism. Micromechanical testing coupled with multiscale confocal microscopy identifies a heterogenous mechanical response in the interface area, endowing the enthesis with a graded response to strains acting from different angles. The presented mechanisms mark a guideline for further biomimetic strategies to rationally design hard-soft interfaces.

CPP 45.2 Wed 15:15 SCH A251

Exposure of leukocytes and hematopoietic stem cells to graphene quantum dots — •Stefan Fasbender[1], Sonja Allani[1], Christian Wimmenauer[1], Patrick Cadeddu[2], Katharina Raba[3], Johannes Fischer[3], Bekir Bulat[4], Claus Seidel[4], Thomas Heinzel[1], and Rainer Haas[2] — [1]Heinrich-Heine-Universität Düsseldorf, Institut für experimentelle Physik der kondensierten Materie — [2]Universitätsklinikum Düsseldorf, Klinik für Hämatologie — [3]Universitätsklinikum Düsseldorf, Institut für Transplantationsdiagnostik — [4]Heinrich-Heine-Universität Düsseldorf, Institut für Molekulare Physikalische Chemie

Fluorescent graphene quantum dots (GQDs) are prepared by the method of Wu et. al [1] via hydrothermal treatment of citric acid and dicyandiamide with subsequent dialysis to obtain a pure GQD solution. The obtained aqueous solution is analyzed with fluorescence spectroscopy, UV-vis, XPS and AFM. Human leukocytes and hematopoietic stem cells are exposed to two different concentrations of GQDs for various times and the uptake dynamic is determined using flow cytometry. A higher uptake is observed into cells with phagocytotic properties. The number of incorporated GQDs is estimated by comparing the fluorescence of cells with GQDs and without GQDs. A permeability constant for the various cell types is calculated and the effect of the GQDs on the viability of the cells is assessed with the XTT viability assay.

[1] Wu et al., Nanoscale, 2014, 6, 3868

CPP 45.3 Wed 15:30 SCH A251

Guanidinium Salts Can both Cause and Prevent the Hydrophobic Collapse of Biomacromolecules — •Jan Heyda[1,2], Halil Okur[3], Joachim Dzubiella[2,4], Pavel Jungwirth[5], and Paul Cremer[3,6] — [1]Physical Chemistry Department, UCT Prague,

Czech Republic — [2]Institut für Weiche Materie und Funktionale Materialien, HZB Berlin, Germany — [3]Chemistry Department, Penn. State University, Pennsylvania, USA — [4]Institut für Physik, HU Berlin, Germany — [5]Institute of Organic Chemistry and Biochemistry, CAS, Prague, Czech Republic — [6]Biochemistry and Molecular Biology Department, Penn. State University, Pennsylvania, USA

A combination of experimental methods with theory and simulations were performed to probe the mechanisms by which guanidinium (Gnd^+) salts influence the stability of the collapsed vs. uncollapsed state of an elastin-like polypeptide (ELP). The Gnd^+ action was found highly dependent upon its counteranion, resulting in three distinct physical regimes. (1) Well-hydrated Gnd_2SO_4 salt was depleted from the ELP/water interface and was found to stabilize the collapsed state of the macromolecule. (2) Salts (e.g. GndSCN), which interacted very strongly with the polymer, stabilized the collapsed state at low salt concentrations, when both ions were found to be enriched in the collapsed state of the polymer. The collapsed state is stabilized due to crosslinking of the polymer chains. At higher salt concentrations, the same strong salt-polymer interaction results in stabilization of the uncollapsed state. (3) GndCl interacted in an intermediate fashion favored the uncollapsed state at all salt concentrations.

CPP 45.4 Wed 15:45 SCH A251

Altering Synthetic Semiexible DNA Nanotube Networks by Tunable Cross-linking — •Martin Glaser[1,2], Paul Mollenkopf[1,2], Christin Möser[2], Carsten Schuldt[1,2], Jörg Schnauss[1,2], Josef Käs[1], and David Smith[2] — [1]Faculty of Physics and Earth Sciences, Institute of Experimental Physics I, Leipzig University, Germany — [2]Fraunhofer Institute for Cell Therapy and Immunology IZI, DNA Nanodevices Group, Germany

The mechanical properties of complex soft matter have been subject to various experimental and theoretical studies. The underlying constituents often cannot be modeled in the classical physical frame of flexible polymers or rigid rods. Polymers in the semiflexible regime, where the finite bending stiffness leads to a non-trivial mechanical contribution, are a highly interesting subclass and can be found in the cytoskeleton of living cells. A natural occurring model system for such polymers is the protein actin. However, experimental studies of actin networks to validate existing theories, are limited since the persistence length cannot be altered. Here, we establish a tunable system of cross-linked, synthetically DNA nanotubes to overcome this limitation. We present first results of the impact tunable cross-linking has on the well-characterized entangled DNA nanotube networks. These studies enable investigations of the impact of a crucial parameter of semiflexible polymers, namely the persistence length, on emerging network properties. Also, the study will allow a deeper insight into the underlying mechanics of biomaterials, such as hydrogels, which are extensively used for in vitro as well as in vivo applications.

CPP 45.5 Wed 16:00 SCH A251

Ion and Molecule Transport in Surface Modified Nanopores - a NMR Study — •Sarah Schneider and Michael Vogel — TU Darmstadt Solid State Physics, Darmstadt, Germany

We analyze ion and molecule transport in surface modified nanopores. It is part of a project that aims to develop a new generation of nanosensors by combining biological and synthetic nanopores. While being highly selective and sensitive, biological ion channels lack the robustness for technological applications. Contrarily silica pores are well-proven in industrial and clinical environments, but possess inferior capabilities, e.g. no selectivity. A hybrid system would combine the favorable properties of both fields.

To optimize such pores, it is of strong interest to understand the influence of this confinement on the ion and molecule transport inside. Such confined dynamics depend on the pore geometry and the guest-host interactions determined by the properties of the inner surfaces.

We vary these parameters systematically, in particular by peptide functionalization of the silica surfaces and study their effects on the dynamics by NMR. This includes various techniques aiming at local dynamics. SFG NMR is applied to measure self-diffusion coefficients of aqueous salt solutions in bulk and nanopore confinement. The experimental setups include ^{1}H and ^{2}H NMR to selectively investigate water dynamics as well as ^{7}Li and ^{23}Na NMR to analyze the diffusion of various ionic species. We find a slowdown of dynamics in confinement. The extent of the effect and the relation between short- and long-range dynamics substantially depends on the confinement properties.

15 min break

CPP 45.6 Wed 16:30 SCH A251

Model-independent measurements of ATP diffusion in PEG-DA hydrogels with various mesh sizes — •Günter Majer[1] and Alexander Southan[2] — [1]MPI für Intelligente Systeme, Heisenbergstr. 3, 70569 Stuttgart, Germany — [2]Institut für Grenzflächenverfahrenstechnik und Plasmatechnologie IGVP, Universität Stuttgart, Nobelstraße 12, 70569 Stuttgart, Germany

Hydrogels are semi-solid polymer networks formed by cross-linked hydrophilic polymer chains, with mesh sizes that can be tailored by varying the concentration and/or the molecular mass of the polymers. Well-defined hydrogels are ideal materials for various applications including drug delivery, transport of nutrients, or devices to separate small molecules chromatographically. In this context, a fundamental understanding of the diffusion processes of solutes in hydrogels with different mesh sizes is important. A powerful tool to determine the diffusion coefficients of solutes directly, i.e. without the need of a fluorescent label and independent of any diffusion-model assumptions, is pulsed field gradient nuclear magnetic resonance (PFG-NMR). In this work, polyethylene glycol diacrylate (PEG-DA)-based hydrogels with mesh sizes ranging from 1.35 to 3.70 nm were prepared using polymers with molecular masses between 700 and 8000 g/mol and concentrations of up to 30%. The diffusion coefficients of adenosine triphosphate (ATP) in these hydrogels were studied by PFG-NMR. The correlation between the mesh sizes and the diffusion coefficients is analyzed and discussed.

CPP 45.7 Wed 16:45 SCH A251

Stress-induced long-range ordering in spider silk — •Johannes Wagner and Frauke Gräter — Heidelberg Institute for Theoretical Studies, Heidelberg, Germany

A range of composite or semi-crystalline materials consist of particles or crystallites embedded randomly in a much softer phase. Emergence of long-range order of these particles within the softer matrix could result in lowering the mechanical energy of the system upon stretching, in consistence with the well-known coalescence of defects in materials. Using small-angle neutron scattering (SANS) and finite element (FE) models we show the presence of such stress-induced ordering in spider silk fibers. Both methods show striking quantitative agreement of the position, shift and intensity increase of the long period upon stretching. We demonstrate that this mescoscopic ordering does not originate from strain-induced crystallization at the atomistic scale, and instead arises from a non-affine deformation that enhances density fluctuations of the two phases along the direction of stress. Our results suggest long-range ordering as a wide-spread phenomenon that can be exploited for tuning the mechanical properties of many hybrid materials with stiff and soft phases.

CPP 45.8 Wed 17:00 SCH A251

Tuning coiled coils mechanically and thermodynamically by histidine-metal coordination — •Isabell Tunn, Kerstin G. Blank, and Matthew J. Harrington — Max Planck Institute of Colloids and Interfaces, Science Park Potsdam Golm, 14424 Potsdam

Coiled coils serve as structural motifs in proteins with mechanical function, such as myosin or α-keratin. In the field of bioinspired materials, naturally occurring and synthetic coiled coils with high binding specificity have become versatile material building blocks, which are used as crosslinkers for hydrogels with applications in cell culture and tissue engineering. Very little is currently understood about the mechanical properties of coiled coils. Yet, this information is critical for controlling and tuning bulk properties of coiled coil-based materials. In order to generate mechanically tunable coiled-coil based materials, metal coordination sites were engineered into a well-characterized heterodimeric coiled coil. Protein-metal coordination bonds are strong, non-covalent interactions mediated by amino acid ligands. Here, two histidine residues were introduced at the coiled coil termini with the goal of stabilizing helical turns. Histidine-metal coordination increased the stability of the coiled coil mechanically and thermodynamically, as demonstrated by AFM single molecule force spectroscopy and CD spectroscopy. We conclude that increasing the stability of single helical turns via metal binding directly affects the overall stability of the coiled coil, providing the potential for generating mechanically tunable biomimetic polymers. Furthermore, these results also provide crucial information about the failure mechanism of coiled coils under load.

CPP 46: Organic Thin Films II (joint session CPP/DS/HL, organized by DS)

Time: Wednesday 15:00–17:00 Location: CHE 91

CPP 46.1 Wed 15:00 CHE 91

Crystallinity and Degradability of Nano- and Microscaled Biopolymer Thin Films — Preetam Anbukarasu[1], Dominic Sauvageau[1], and •Anastasia Elias[1,2] — [1]Chemical and Materials Engineering, University of Alberta, Edmonton, Canada — [2]Leibniz-Institut für Polymerforschung Dresden e. V.

Enzymatically-degradable polymer thin films are attractive for biomedical, packaging, micro-electronic and agricultural applications. The stability and degradability of these materials are known to depend on both the parameters under which they are processed, and on the environmental conditions under which degradation occurs. Processing conditions are especially relevant for semi-crystalline polymers, since the degree of crystallinity of a material is an important determinant of its degradability.

In this work, we examine the effect of nano-scale dimensional constraint on the crystallinity and enzymatic degradability of polyhydroxybutyrate (PHB), a biopolymer. The physical properties of solution-cast PHB films of varying thicknesses were examined by atomic force microscopy (AFM, lamella orientation & surface profile) and x-ray diffraction (XRD, crystallinity & crystal anisotropy). The enzymatic degradability was tested using a diffraction grating-based optical sensor. We found that as the thickness of the samples was reduced from 5 um to less than 100 nm, the crystallinity of the films decreased, while the rate of degradation increased. However, below 100 nm, surprisingly slow degradation rates were observed. This occurs due to the fact that these films are amorphous, inhibiting the binding of the enzymes.

CPP 46.2 Wed 15:15 CHE 91

Determination of the molecular orientation in absorptive organic thin films — •Christian Hänisch, Simone Lenk, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics

The overall efficiency of organic light-emitting diodes (OLEDs) is mainly limited by the high refractive index of the organic layers causing a trapping of large portions of the initially emitted light. Using emitter molecules with transition dipole moments parallel to the interface planes of an OLED reduces this loss channel and hence, increases the outcoupling efficiency of the device. The orientation of the molecules' transition dipole moments can be determined by angular resolved photoluminescence spectroscopy.

We investigate the impact of the organic layer's absorption on the determined orientation value by evaluating the emission spectra of single organic layers with thicknesses up to 150 nm. Numerically, these emission layers are represented by a set of radiating electrical dipoles which are homogeneously distributed over the whole layer. To represent the absorption of the excitation light, the single dipoles are weighted by an exponential function according to the Beer-Lambert law.

Using this method, we can show that the orientation parameter of the red phosphorescent emitter Ir(MDQ)$_2$(acac) doped into NPB is stable over a time range of several months at temperatures between room temperature and 80°C which is only 5% below the glass transition temperature of NPB.

CPP 46.3 Wed 15:30 CHE 91

Interface-Controlled DNTT Thin Films: Growth, Morphology, and Temporal Evolution — •Andrea Karthäuser[1], Tobias Breuer[1], Hagen Klemm[2], Francesca Genuzio[2], Gina Peschel[2], Alexander Fuhrich[2], Thomas Schmidt[2], and Gregor Witte[1] — [1]FB Physik, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Abt. Chemische Physik, FHI der MPG, 14195 Berlin, Germany

The high charge carrier mobility and chemical stability of dinaphthothienothiophene (DNTT) render this new organic semiconductor (OSC) especially interesting for organic field effect transistors (OFETs) [1, 2]. Despite such device advances, the structure and morphology of DNTT thin films are so far rather unexplored. On the prototypical substrates SiO$_2$ and graphene we prove a substrate-mediated control of the molecular orientation by means of NEXAFS and XRD measurements. Furthermore, by using atomic force microscopy (AFM) and photoelectron emission microscopy (PEEM) we analyzed the morphology of DNTT films with variable thicknesses and find a temporal dewetting of these films. This pronounced island formation leads to a breakup of the film which is most efficient for thin films of a few monolayers. Finally we have extend this study also to device relevant substrates by analyzing DNTT films that were grown on SAM treated dielectrics. Again a district dewetting is found, which is expected to affect the long-term performance of DNTT devices and appears surprising in view of the reported long term stability of DNTT-OFETs [2].

[1] Yamamoto, T.; J. Am. Chem. Soc. (2007), 129,224. [2] Zschieschag, U.; Org. Electron. (2013), 14, 1516.

CPP 46.4 Wed 15:45 CHE 91

Direct photo alignment and optical patterning: Controlling molecular thin film growth on the meso-scale — •Linus Pithan[1,3], Paul Beyer[1], Laura Bogula[1], Anton Zykov[1], Peter Schäfer[1], Jonathan Rawle[2], Chris Nicklin[2], Andreas Opitz[1], and Stefan Kowarik[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Berlin, Germany — [2]Diamond Light Source, Didcot, UK — [3]ESRF, Grenoble, France

A novel strategy for direct photoalignment of molecular materials using optothermal re-orientation is introduced. We show that it is possible to fabricate anisotropic and photolithographically patterned organic molecular thin films based on light-directed molecular self-assembly (LDSA).[1]

Growing tetracene thin films via LDSA on amorphous silica, we employ 532 nm laser illumination, which matches the lower Davydov absorption band, to induce preferential orientations of molecular crystal grains. Based on grazing incidence X-ray diffraction (GIXD) as well as optical spectroscopy we determine a threshold laser power for azimuthal alignment. The patterning and polarized light emission that is possible with LDSA is important for applications such as polarized organic light emitting diodes or photonic metasurfaces.

[1] L. Pithan et. al. Adv. Mater. doi:10.1002/adma.201604382

CPP 46.5 Wed 16:00 CHE 91

Modern *in situ* real-time X-ray scattering and nucleation theory for an enhanced understanding of molecular self-assembly — •Anton Zykov[1], Sebastian Bommel[1,2], Yves Garmshausen[3], Linus Pithan[1,4], Paul Beyer[1], Gonzalo Santoro[5], Stefan Hecht[3], Jürgen P. Rabe[1], and Stefan Kowarik[1] — [1]Inst. f. Physik, Humboldt-Universität zu Berlin — [2]DESY, Hamburg — [3]Inst. f. Chemie, Humboldt-Universität zu Berlin — [4]ESRF, Grenoble, France — [5]Inst. de Ciencia de Materiales de Madrid, CSIC, Spain

Quantifying nanoscale processes that drive the self-assembly of organic molecules into functional thin films is the prerequisite to understand and steer structure formation. In a study on the growth of PTCDI-C$_8$ we unravel a remarkable layer-dependent molecular diffusion behaviour from an innovative simultatineous *in situ* acquisition of X-ray reflectivity growth oscillations and diffusively scattered X-rays and the application of state-of-the-art nucleation theory. This allows us to determine nucleation energies, critical cluster sizes and attempt frequencies.[1] These quantities can be strongly influenced when applying chemical tuning to well-known molecules. We showcase this on the example of the growth of 6P and 6PF2. As a result of the fluorination we achieve a significant film smoothening as desired for applications, where an efficient in-plane charge carrier transport is of importance.

[1]A. Zykov *et al.*, J. Chem. Phys. 146, 052803 (2017)

CPP 46.6 Wed 16:15 CHE 91

Modeling of singlet fission in weakly-interacting acene molecules — Sharareh Izadnia[1], David W. Schönleber[2], •Alexander Eisfeld[2], Alexander Ruf[1], Aaron C. LaForge[1], and Frank Stienkemeier[1] — [1]Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden

Singlet fission, a process in which a singlet excited state is converted into two triplet states, is a means to circumvent the Shockley-Queisser limit for energy conversion in solar cells. In a recent experiment, singlet fission was observed in a disordered system where organic chromophores are distributed on the surface of a rare gas cluster. Here we give details on the theoretical modeling of singled fission in this system. Our kinematic model explicitly takes into account the details of the geometrical arrangement of the system as well as the time-dependent populations of the relevant states of each molecule. Using this model, which goes beyond usual mean-field treatment, we study the trends obtained by singlet fission, exciton-exciton annihilation, and singlet hopping on the experimental observables. Our simulations support the conclusion of the experimental observation that SF is present even at weakly interacting conditions.

CPP 46.7 Wed 16:30 CHE 91

Ultra-robust thin film devices from metal-terpyridine wires — •Florian von Wrochem[1], Maria Anita Rampi[2], and Wolfgang Wenzel[3] — [1]Materials Science Laboratory, Stuttgart — [2]Dipartimento di Chimica, Universita' di Ferrara — [3]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany

Considerable efforts have been undertaken within the past decades to shift organic-based thin-film devices from basic research to the application level. A major hurdle is given by the thermal deposition of the metal electrodes, which remained elusive due to the damage and the electrical shorts experienced by the fragile molecular layers. Here, we show that large area molecular junctions of outstanding electronic properties and robustness can be realized using densely packed molecular wires consisting of FeII-terpyridine complex oligomers, despite a conventional fabrication process involving top electrode evaporation directly on the molecular layer. Surprisingly, these oligomer-based devices are stable for over 2 years under regular current-voltage cycling, withstanding a wide range of temperatures (150-360 K) and applied voltages (3 V). Electrical studies in conjunction with ab-initio calculations reveal that charge transport (i) occurs via electron (hopping) conduction and is limited by the charge injection through a Shottky barrier (0.72 eV), following Richardson-Schottky injection.

CPP 46.8 Wed 16:45 CHE 91

Superradiance from two dimensional brick-wall aggregates of dye molecules: the role of size and shape for the temperature dependence — •Alexander Eisfeld[1], Christian Marquardt[2], and Moritz Sokolowski[2] — [1]MPI-PKS — [2]Uni Bonn

Aggregates of interacting molecules can exhibit electronically excited states which are coherently delocalized over many molecules. This can lead to a strong enhancement of the fluorescence decay rate which is referred to as superradiance (SR). To date, the temperature dependence of SR is described by a $1/T$ law. Using an epitaxial dye layer and a Frenkel-exciton based model we provide both experimental and theoretical evidence that significant deviations from the $1/T$ behaviour can occur for brickwall-type aggregates of finite size leading even to a maximum of the SR at finite temperature. This is due to the presence of low energy excitations of weak or zero transition strength.

CPP 47: Fluids and Interfaces I

Time: Wednesday 16:15–18:15 Location: ZEU 255

Invited Talk CPP 47.1 Wed 16:15 ZEU 255

Hard science with soft spheres: learning from foams and emulsions — •Wiebke Drenckhan-Andreatta — Institut Charles Sadron, CNRS UPR22, Srasbourg, France

Who has not marvelled at the delicate organisation of bubbles floating on top of a beer or a bathtub? Or similarly, of oil drops hovering on the surface of a soup or a vinaigrette? Under gravity, those soft and frictionless bubbles and drops snuggle neatly together, creating sphere-type packings where the influence of gravity is small, and polyhedral packings, where the influence of gravity is important.

Being able to understand and to predict these packings has challenged physicists and mathematicians alike; and their close collaboration has brought forward an increasingly deep understanding of the intriguing features that characterise the packing procedures and the final structure of foams and emulsions.

Building on these advances, physical chemists are now joining this subject. The necessity of stabilising foams or emulsions with interfacially active agents (soap-like molecules, block-copolyers, particles,...), provides a vast playground to tune (and to understand) the interactions of these soft spheres via specific modifications of their surfaces: How do the interactions change if the bubbles/drops are covered by a visco-elastic skin? How to they pack if this skin creates non-negligible friction? And what if these spheres are adhesive?

In this presentation I will give an overview of the state of the art of this interdisciplinary field in bridging historical aspects with recent findings.

CPP 47.2 Wed 16:45 ZEU 255

The role of aggregates in the stabilization of protein foams — •Manuela E. Richert and Björn Braunschweig — Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster, Germany

Native and fluorescein isothiocyanate (FITC) labelled bovine serum albumin (BSA) were used to investigate the role of protein aggregates in the stabilization of aqueous protein foams through structure-property relations that reach from the molecular to the macroscopic scale. Protein modified air/water interfaces, which are ubiquitous in aqueous foam, were studied with tensiometry and vibrational sum-frequency generation (SFG). At the air/water interface, SFG and tensiometry provide information on coverage and the net charging state of the interface and thus information on the isoelectric point (IEP) of labelled and native BSA proteins at the air/water interface is gained. At the interfacial IEP a reversal of the phase of OH stretching bands from interfacial H_2O molecules is observed in SFG spectra and corresponds to a minimum in the surface tension. The latter can be attributed to the formation of protein aggregates at the interface which promotes macroscopic foam stability. Using confocal fluorescence microscopy aggregates of labelled proteins are found to be predominantly located inside foam lamella where they possibly form a gel-like network and thus cause non-DLVO like interactions.

CPP 47.3 Wed 17:00 ZEU 255

Ultra-thin Polymer Films at the Air/Water Interface: Lateral and vertical structure of poly (butyl acrylate) during compression — •Christian Appel and Bernd Stühn — Institut für Festkörperphysik, Technische Universität Darmstadt, D-64289 Darmstadt, Germany

The behaviour of poly (butyl acrylate), PBA, spread readily at the a/w interface is well studied. It forms stable films that become elastic at high surface pressures (20-30 mN/m).[1] We prepare Langmuir monolayers of PBA and the diblock copolymer poly(ethylene glycol)-PBA with different molecular weights from 5 kg/mol to 20 kg/mol. The PEG block acts as a small hydrophilic anchor ($N_M < 10$).

We perform in-situ Brewster-Angle-Microscopy (BAM) and in-situ X-Ray reflectometry (XRR) to get a thorough understanding of the film structure. For the dilute and semi-dilute regime the surface pressure and coverage follows the expected scaling laws. In the concentrated regime there is a transition from a continuous water-free monolayer to a more complex structure. At first in the semi-dilute regime, XRR and BAM show a single monolayer structure of the film. During the compression to the concentrated regime the lateral structure of the film changes to 2D-disks of PBA within the monolayer. This is complementarily observed by XRR (Yoneda peak and off-specular intensity) and BAM. Hysteresis experiments indicate that a part of the monolayer is irreversible deformed within the concentrated regime.

[1] K. Witte et al., Macromolecules 43, 2990-3003 (2010)

CPP 47.4 Wed 17:15 ZEU 255

Influence of Surfactant Chain Length on the Interfacial Structure and Properties of Surfactant/Polyelectrolyte Mixtures — •Felix Schulze-Zachau and Björn Braunschweig — Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

Mixtures of poly(sodium 4-styrenesulfonate) (NaPSS) polyelectrolytes and 0.1 mM alkyltrimethylammonium bromides C_{16}TAB, C_{14}TAB and C_{12}TAB surfactants were studied at the air/water interface with tensiometry, ellipsometry and vibrational SFG spectroscopy as a function of PSS concentration. In addition, macroscopic foams from these mixtures were studied in order to relate the interfacial molecular structure and its charging state to foam stability. ζ-potential and turbidity measurements were done to investigate charge and equilibrium states of the respective systems in the bulk solution. The chemical potential of the surfactants to bind to PSS increases with their chain length, which results in different interfacial structures. For C_{16}TAB, charge neutralization in the bulk and at the interface is observed close to equimolar concentrations and leads to bulk solutions that are far outside the thermodynamic equilibrium. Here, hydrophobic complexes aggregate and precipitate for C_{16}TAB while binding to PSS is much weaker for C_{14}TAB and C_{12}TAB where no precipitation is observed. In case of C_{16}TAB/PSS mixtures, SFG spectra indicate a phase shift of the water molecules that is indicative for a charge reversal at the interface at 0.09 mM. Complementary methods indicate a depletion of complexes from the interface when this point of zero charge is crossed.

CPP 47.5 Wed 17:30 ZEU 255

Tuning protein adsorption using multivalent ions — •Madeleine Fries[1], Frank Schreiber[1], Fajun Zhang[1], Alexander Hinderhofer[1], Robert Jacobs[2], and Maximilian Skoda[3] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — [2]Chemistry Research Laboratory, University of Oxford, Oxford, OX1 3TA, United Kingdom — [3]Rutherford-Appleton Laboratory, ISIS Facility, Didcot, OX11 0QX, United Kingdom

We studied protein (bovine serum albumin, BSA) adsorption at the solid-liquid interface tuned by trivalent ions (Y^{3+}) using ellipsometry, neutron reflectivity and quartz-crystal microbalance. We find re-entrant behavior of the interface adsorption, which increases upon approaching c* and decreases above c**, where c* and c** are the corresponding critical concentrations marking the region of the re-entrant condensation behavior in the bulk. We thus manage to relate the rich bulk phase behavior, which also features liquid-liquid phase separation and new pathways to crystallization [1] discussed in terms of an ion-activated attractive patch model [2], to the interface adsorption behavior. In addition to the general challenge of connecting bulk and interface behavior, our work has implications for, inter alia, nucleation at interfaces.

[1] Zhang, F.et. al, Physical Review Letters 2008, 101 (14), 148101.

[2] Roosen-Runge, F.; Zhang, F.; Schreiber, F.; Roth, R., Scientific reports 2014, 4, 7016.

CPP 47.6 Wed 17:45 ZEU 255

Solvent Extraction: Structure of the Liquid-Liquid Interface Containing a Diamide Ligand — •Ernesto Scoppola[1], Erik Watkins[2], Richard Campbell[3], Oleg Konovalov[4], Luc Girard[5], Ignacio Rodriguez-Loureiro[1], Jean-François Dufrêche[5], Geoffroy Ferru[6], Giovanna Fragneto[3], Emanuel Schneck[1], and Olivier Diat[5] — [1]Max Planck Institut of Colloids and Interfaces, Potsdam, Germany — [2]LANL, Los Alamos, USA — [3]ILL, Grenoble, France — [4]ESRF Grenoble, France — [5]ICSM, Bagnols sur Cèze Cedex, France — [6]ANL, Lemont, USA

Knowledge of the (supra)molecular structure of an interface that contains amphiphilic ligand molecules is necessary for a full understanding of ion transfer during solvent extraction. Even if molecular dynamics simulations already yield some insight in the molecular configurations in solution, hardly any experimental data giving access to distributions of both ligands and ions at the liquid*liquid interface exist. Here, the combined application of X-ray and neutron reflectometry represents a milestone in the deduction of the interfacial structure and potential with respect to different lipophilic ligands. It is also shown that neutron reflectometry can specifically reveal the ion distribution at the interface when neutron absorption and neutron-induced gamma-fluorescence are analyzed. To this end we show that hard trivalent cations can be repelled or attracted by the ligand-enriched interface depending on the nature of the ligand. References: 1.Scoppola E et al. (2016) Solvent Extraction: Structure of the Liquid-Liquid interface containing a Diamide ligand. Angewandte Chemie International Edition 55 (32), 9326.

CPP 47.7 Wed 18:00 ZEU 255

Light-switchable molecules at planar fluid interfaces — •Josua Grawitter and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany

Surfactants are part of many self-assembled structures in soft matter, from biological membranes to liquid foams. Especially promising are surfactants which change shape under illumination, so-called *photosensitive surfactants*, because their isomer densities can locally be manipulated with light.

We study their dynamics at a planar fluid interface using a coarse-grained theory for a surfactant mixture, which follows previous research on surfactant-driven droplets [1, 2]. The theory takes into account light-switching, surfactant adsorption, diffusion, mean field interactions, and advection due to Marangoni flow, which is initiated by gradients in surface tension. We present an exact solution of the incompressible Stokes flow for two immiscible fluids with an arbitrary field of surface tension at a planar interface. Using our theory we calculate the dynamic profiles of photosensitive surfactants driven by spots of light with intensities either constant in time or oscillating.

[1] M. Schmitt and H. Stark, Europhys. Lett. **101**, 44008 (2013).

[2] M. Schmitt and H. Stark, Phys. Fluids **28**, 012106 (2016).

CPP 48: Poster: Polymer Crystallization, Nucleation and Selfassembly

Time: Wednesday 18:30–21:00 Location: P2-OG1

CPP 48.1 Wed 18:30 P2-OG1

On the controvercy close folds versus coils in polyethylene and the weight of evidence. — •Heinz H.W. Preuss — Hameln

The highest weight of evidence in the field of morphology belongs to direct visualization and photography. Results of direct visualization and photography of entangled and coiled or looped chains of polymeric molecules in melts and of close folds of chains in solid polymers are not yet found to be published. But separated lamellae of HDPE could be visualized and photographed by H. Preuss (1) with a TEM after tearing them off from the surface of a specimen solidified from melt by slow cooling. The thickness of the lamellae (120 nm) was estimated from the shadow length in the fracture surface after evaporation of carbon under a 30o angle, and the orientation of the chains perpendicular to the plane of the lamellae was confirmed by electron diffraction. Thus the fold model of A. Keller could be confirmed as sure as for polyethylene crystals from dilute solution. *When the lamellae are isolated single entities, as in solution crystallization then given that the chains are perpendicular, or at a large angle to the basal plane, folding is a straightforward necessity as the chains have nowhere else to go."(2) Entangled and coiled molecules remain a fiction until they would be observed directly. 1 - H.H.W.Preuss, physica status solidi, vol. 3, 1963, K 109 ff.; Plaste und Kautschuk, 22.Jg. Heft 12, 1975, 958-959 2 - A. Keller, Faraday Discussion 1979 p. 149

CPP 48.2 Wed 18:30 P2-OG1

NMR investigations of dynamics in the different phases of semicrystalline polymers — •Mareen Schäfer, Ricardo Kurz, Martha Schulz, Anne Seidlitz, Thomas Thurn-Albrecht, and Kay Saalwächter — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale), Germany

The melt-crystallized morphology of semicrystalline polymers strongly depends on the diverse dynamics in the amorphous and crystalline region. The connections between structure formation and dynamics of polymer chains are investigated with SAXS and NMR spectroscopy, respectively, and polymers with and without intracrystalline dynamics (crystal-mobile and crystal-fixed) are compared. Proton time-domain techniques enable the analysis of the phase components, the intracrystalline and the amorphous phase dynamics. The intracrystalline motion displays only a weak dependence on morphology. SAXS results show that the morphology of the crystal-fixed polymer, poly-ϵ-caprolactone (PCL), and the crystal-mobile polymer, polyethylene oxide (PEO), are qualitatively different. The crystal thicknesses in PCL are well-defined whereas in PEO a crystal reorganization process caused by the intracrystalline dynamics leads to a uniform amorphous region. To investigate the impact of the crystalline growth and reorganization process on the morphology separately, polymers with slower intracrystalline mobility, e.g. polyoxymehtylene (POM), will be investigated. Further investigations address the relationship between morphology and entangled dynamics in the amorphous phase.

CPP 48.3 Wed 18:30 P2-OG1

Molecular Dynamics simulations of deformation induced solubility of poly(ethylene oxide) in water — •Sergii Donets[1], Olga Guskova[1], and Jens-Uwe Sommer[1,2] — [1]Insitute Theory of Polymers, Leibniz-Institute of Polymer Research, D-01069 Dresden, Germany — [2]Technische Universität Dresden, Institute for Theoretical Physics, D-01069 Dresden, Germany

Metastability of hydrated polymer solutions can lead to a spontaneous solidification via H-bonding in response to the stress fields, e.g. under flow conditions. This could potentially help to overcome the problem of high energy input at each stage of the processing path and provide us with low energy, wet-processing techniques for producing sustainable polymeric materials. Water solution of poly(ethylene oxide) is considered as a potential candidate capable of undergoing the phase transition as a result of loss of the hydrated structure. We have performed classical molecular dynamics simulations to study thermodynamic and structural properties of poly(ethylene oxide) under deformation in water.

CPP 48.4 Wed 18:30 P2-OG1

Effects of the α_c-relaxation for PEO and POM: Impact on Crystallization Process, Morphology and Reorganization Behavior — •Martha Schulz, Anne Seidlitz, and Thomas Thurn-Albrecht — Institute of Physics, MLU Halle-Wittenberg, Germany

Depending on the presence or absence of an α_c-relaxation it is possible to distinguish between crystal-mobile and crystal-fixed semi-crystalline polymers. Only crystal-mobile polymers own a certain chain mobility in the crystalline phase. In contrast to the crystal-fixed polymer Polycaprolactone (PCL), we analyze the impact of the α_c-relaxation for two representatives of α_c-mobile polymers, Polyethylenoxide (PEO) and Polyoxymethylene (POM), using different methods like SAXS and Flash-/DSC.

SAXS-measurements show that crystal-fixed polymers follow the expectations of classical crystallization theories. The crystal thickness is determined by the crystallization temperature Tc. In contrast the crystal-mobile polymers shows a thickening of the crystalline lamellae up to a minimal thickness of the amorphous regions, enabled trough the α_c-relaxation. As a consequence, crystal-mobile and crystal-fixed polymers exhibit a different reorganization behavior during heating. The crystallization of PCL leads to the formation of marginally stable crystallites which constantly reorganize during heating, while in PEO and POM due to the presence of the α_c-relaxation, much more stable (thickened) lamellar crystals form, which melt only at much higher temperatures. Crystallization at low temperatures on the other hand seems to suppress the α_c-induced stabilization also in PEO.

CPP 48.5 Wed 18:30 P2-OG1

Separated lamellae of HDPE solidified from melt by slow cooling. — •Heinz H.W. Preuss — Hameln

The poster shows a representative selection of TEM photographs of mechanically separated lamellae of HDPE by H. Preuss (1). The specimen was heated in an oven and held for 20 minutes at 200 degrees centigrade, cooled down to 100 degrees centigrade in 30 minutes (3 K/min). The free surface was covered with a thin layer of gold (20 nm) by evaporation in vacuum. The gold layer was thickened with Cu by galvanization (0,1 mm). The metal sheet was torn off and the surface covered with C by evaporation in vacuum under an angle of nearly 30o. Then the copper was resolved with nitric acid and the gold after addition of hydrochloric acid. The C layer was put in the TEM on a grid woven with bronze wire. In the TEM one could see lamellae of polyethylene attached at the C layer showing the relief of the fracture surface by shadowing. The orientation of the molecular chains perpendicular to the plane of lamellae cold be confirmed by electron diffraction. Thus the chain folding model of A. Keller (2) cold be confirmed for HDPE solidified from the melt. 1. H.H.W.Preuss, physica status solidi Nr. 3 1963, 109 K ff; Plaste und Kautschuk 22. Jg. Heft 12/1975, 258 f. 2. 2. A. Keller, Kolloidzeitschrift, 165, 3 (1959)

CPP 48.6 Wed 18:30 P2-OG1

Crystallization of polymers studied by combining AFM and fast scanning calorimetry — •Rui Zhang, Evegny Zhuravlev, and Christoph Schick — Institute of Physics, University of Rostock, Albert-Einstein-Str. 23-24, 18051 Rostock, Germany and Competence Centre CALOR, Faculty of Interdisciplinary Research, University of Rostock, Albert-Einstein-Str. 25, 18051 Rostock, Germany

Atomic force microscopy (AFM) can show morphology of polymers at the early stages of crystallization (structures on a 100 nanometer scale). In combination with fast scanning calorimetry (FSC), AFM can detect polymer crystallization after fast quenches and after short annealing (sub second). The calorimetric chip sensor is mounted on the AFM and the fast scanning calorimetric measurements are possible without touching the sensor. This way a repeated heat treatment of the sample is possible and the formed structures are accessible for the AFM at room temperature if the glass transition temperature of the polymer is above room temperature. The primary results show morphologies after deep quenches in the homogeneous nucleation domain and for low supercooling in the heterogeneous nucleation domain. The spherulitic growth rates at high temperatures have been determined, which are faster than POM's data given by others.

CPP 48.7 Wed 18:30 P2-OG1

Formation of periodically modulated single crystals of isotactic polystyrene — •Purushottam Poudel, Sumit Majumder, and Günter Reiter — Physikalisches Institut, Albert-Ludwigs- Universität Freiburg, Hermann-Herder-Straße 3, D-79104 Freiburg, Germany

Polymer crystals are often composed of stacks of lamellae, separated by amorphous layers. The underlying mechanism of self-induced nucleation of secondary lamellae is at the origin of crystal growth in the direction of the surface normal of the lamellae, generating three-dimensional (3-D) stacks of lamellar crystal. In order to explore such growth of 3-D crystals consisting of correlated lamellae, we have chosen thin films of isotactic polystyrene. Interestingly, we observed the formation of periodically modulated crystalline structures consisting of stacks of correlated lamellae. The spacing between such stacks, i.e. the period, was found to increase with increasing crystallization temperature and film thickness. Detailed investigations via atomic force microscopy revealed that the periodically modulated structures resulted from the interplay between nucleation of stacks of secondary lamellae, growth of these lamellae and diffusion of polymer chains.

CPP 48.8 Wed 18:30 P2-OG1

Evidence for self-organized formation of logarithmic spirals during explosive crystallization of amorphous Ge:Mn layers — •Danilo Bürger[1], Stefan Baunack[2], Jürgen Thomas[3], Steffen Oswald[3], Horst Wendrock[3], Lars Rebohle[4], Thomas Schumann[4], Wolfgang Skorupa[4], Daniel Blaschke[4], Thomas Gemming[3], Oliver G. Schmidt[1,2], and Heidemarie Schmidt[1] — [1]Material Systems for Nanoelectronics, Chemnitz University of Technology, Chemnitz 09126, Germany — [2]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstraße 20, Dresden 01069, Germany — [3]Institute for Complex Materials, IFW Dresden, Helmholtzstraße 20, Dresden 01069, Germany — [4]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, P.O. Box 510119, 01314 Dresden, Germany

Logarithmic spirals are found on different length scales in nature, e.g. in nautilus shells, cyclones, and galaxies. The underlying formation laws can be related with different growth mechanisms, pressure gradients, and density waves. Here we report on the self-organized formation of symmetric logarithmic crystallization spirals in a solid material on the micrometer length scale, namely in an amorphous Ge:Mn layer on a Ge substrate. After exposure to a single light pulse of a flashlamp array, the Ge:Mn layer is crystallized and reveals a partially rippled surface and logarithmic microspirals. Finally, we present a model describing the formation of the crystallization spirals by directional explosive crystallization of the amorphous Ge:Mn layer which is triggered by the flashlamp light pulse.

CPP 48.9 Wed 18:30 P2-OG1

Investigating crystal-liquid interface by using fundamental measurement theory — •ShangChun Lin and Martin Oettel — Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany

The crystal-liquid interface is important in material science. For the crystal-liquid interface, fundamental measure theory (FMT) within density functional theory (DFT) provides the almost accurate description of the hard-sphere system. In FMT, the equilibrium crystal-liquid interface has been evaluated within DFT, but has not been tackled within dynamic density functional theory (DDFT). The dynamics play a crucial role in non-equilibrium systems, such as nucleation. Thus, we developed a semi-empirical cut-off method to stabilize single crystals and the crystal-liquid interface. The results are in a good agreement with FMT within DDFT. The free energy difference is less than $10^{-4}k_BT$ for the crystal phase near crystal-liquid coexistence and surface tensions compare well with previous results from DFT. Also, preliminary results for crystals and interfaces in the Asakura-Oosawa model are presented.

CPP 48.10 Wed 18:30 P2-OG1

Investigating crystal-liquid interface by using fundamental

measurement theory — •ShangChun Lin and Martin Oettel — Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany

The crystal-liquid interface is important in material science. For the crystal-liquid interface, fundamental measure theory (FMT) within density functional theory (DFT) provides the almost accurate description of the hard-sphere system. In FMT, the equilibrium crystal-liquid interface has been evaluated within DFT, but has not been tackled within dynamic density functional theory (DDFT). The dynamics play a crucial role in non-equilibrium systems, such as nucleation. Thus, we developed a semi-empirical cut-off method to stabilize single crystals and the crystal-liquid interface. The results are in a good agreement with FMT within DDFT. The free energy difference is less than $10^{-4}k_BT$ for the crystal phase near crystal-liquid coexistence and surface tensions compare well with previous results from DFT. Also, preliminary results for crystals and interfaces in the Asakura-Oosawa model are presented.

CPP 48.11 Wed 18:30 P2-OG1

The role of trivalent salts in protein nucleation and crystallization — •Marcus Mikorski[1], Andrea Sauter[1], Fajun Zhang[1], Benedikt Sohmen[1], Ralph Maier[1], Georg Zocher[2], Thilo Stehle[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — [2]IFIB, Tübingen, Germany

Crystal structures of proteins are essential for understanding protein function. However, crystallography of proteins depends on high quality crystals for diffraction and is therefore often a challenging task. Using the negatively charged protein human serum albumin, we developed a model system to study nucleation and crystallization pathways via theoretical modelling and SAXS and SANS meassurements. We found that in a reentrant condensation state diagram, for negatively charged globular proteins, there are two boundaries at which the probability for high quality crystals is high. Between these boundaries a phase separated regime occurs [1]. This interaction can be tuned by using different trivalent salts ($\mathrm{YCl_3}$, $\mathrm{LaCl_3}$, $\mathrm{CeCl_3}$, $\mathrm{GdCl_3}$) and varying the solvent (D_2O, H_2O). Here, we present data on the influence of these salts on the effective protein-protein interactions and the phase behavior, the pathways of crystal growth and finally the location of metal ions in the crystal unit cell and their role in stabilizing the crystal structure. Crystals grown in different salt and solvent conditions have the same unit cell. Thereby we provide a toolbox for growth of high quality protein crystals for diffraction.

[1] Zhang et al. Pure & Appl. Chem. 2014, 86, 191-202

CPP 48.12 Wed 18:30 P2-OG1

Self-assembly of Partially Fluorinated Hexabenzocoronene Derivatives in the Solid State — •Tobias Breuer[1], Michael Klues[1], Pauline Liesfeld[2], Andreas Viertel[2], Matthias Conrad[1], Stefan Hecht[2], and Gregor Witte[1] — [1]Philipps-Universität Marburg, Germany — [2]Humboldt-Universität Berlin, Deutschland

Fluorination of polycyclic aromatic hydrocarbons (PAHs) is a wellestablished method to enhance the stability of organic semiconductors (OSCs) and render them n-type. For hexabenzocoronene (HBC) it has been observed that fluorination leads to a modification of the molecular packing motif from a herringbone arrangement to a parallel-packed motif. Here, we study whether this transformation of the molecular packing is also found for newly synthesized, partially fluorinated HBCs. Combining powder diffraction and NEXAFS dichroism measurements, we reveal that indeed all partially fluorinated compounds adopt a parallel molecular packing, hence maximizing the intermolecular contact area. We identify fluorine-hydrogen bonds as mediating driving force to stabilize this molecular arrangement. Furthermore, we show that the relative orientation of the HBCs on the underlying surface can be precisely controlled by varying substrate materials. Finally, the energetic states of the compounds are analyzed by photoelectron spectroscopy, optical spectroscopy and DFT to identify the effects of fluorination on these fundamental electronic characteristics.

[1] T. Breuer et al., PCCP, 2016, DOI: 10.1039/C6CP06126E

CPP 48.13 Wed 18:30 P2-OG1

Generating network structures with long-range order in triblock terpolymer films by controlled solvent vapor annealing — •Karolina Korzeb[1], James A. Dolan[2], Ullrich Steiner[1], and Ilja Gunkel[1] — [1]Adolphe Merkle Institute, Fribourg, Switzerland — [2]University of Cambridge, Cambridge, United Kingdom

Triblock terpolymers are an interesting class of polymers due to their potential to self-assemble into a variety of continuous network structures. Amongst these network structures the gyroid is of particular interest. Due to its unique geometry, a gyroid-structured plasmonic material exhibits interesting optical properties, e.g. linear dichroism. While triblock terpolymers were shown to serve as templates for the fabrication of a nanostructured gold gyroid, the anisotropic optical properties related to the gyroid morphology became only evident for samples showing large individual gyroid grains. However, the fabrication of polymer templates with long-range lateral order still remains a challenge. In this work, we show that continuous network structures with long-range lateral order can be generated by means of controlled solvent vapor annealing of a PI-b-PS-b-PGMA (ISG) triblock terpolymer film. In-situ GISAXS was used to identify the regime where films swollen in THF vapor exhibit well-ordered morphologies. The degree of order in these swollen films was maintained only after controlled solvent removal. In this way, grains of about $10\ \mu m$ in size were produced in dry ISG films as determined by AFM Moiré patterns. These films are therefore very promising candidates for the fabrication of gyroid-structured plasmonic materials.

CPP 49: Poster: Surfaces, Interfaces, Thin Films, Nanostructures

Time: Wednesday 18:30–21:00 Location: P2-OG1

CPP 49.1 Wed 18:30 P2-OG1

3D Depth Profiles of the Tip-Sample Interaction on Compliant Polymers — •Martin Dehnert and Robert Magerle — Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Germany

Attractive forces between the tip of an atomic force microscope and a polymer melt or a swollen polymer act over several tens of nanometers. The tip indentation into these compliant materials is of similar size. Both effects cause a large uncertainty in height measurements. Here we compare 3D depth profiles of the tip-sample interaction measured with force-distance (FD) and amplitude-phase-distance (APD) measurements. In particular, we compare the height profiles reconstructed from different characteristic points on FD and APD curves that might characterize the unperturbed surface position: (a) the onset of attractive forces, (b) the contact point where attractive and repulsive forces balance each other, and (c) the position of the maximal attractive force in FD measurements. All three geometrical quantities do not require assumptions about material properties or a specific contact model. As examples, we study polystyrene melts with low molecular weight and polystyrene droplets swollen in solvent vapor. A solid Si wafer serves as substrate and height reference. Our approach allows for accurate height and 3D shape measurements of compliant polymeric nanostructures.

CPP 49.2 Wed 18:30 P2-OG1

Annealing of Diblock Copolymer Thin Films using Solvent Vapor Mixtures — •Florian Jung[1], Anatoly V. Berezkin[1], Detlef-M. Smilgies[2], Dorthe Posselt[3], and Christine M. Papadakis[1] — [1]Technical University of Munich, Physics Department, Garching, Germany — [2]Cornell University, CHESS Wilson Lab, Ithaca, NY, U.S.A. — [3]Roskilde University, Department of Science and Environment, Denmark

Block copolymers self-assemble into nanostructures. Solvent vapor annealing (SVA) is an efficient method to improve the long-range order or to alter the morphology in block copolymer thin films.

In the present work, SVA is carried out on thin films from a polystyrene-b-poly(dimethyl siloxane) (PS-b-PDMS) diblock copolymer. For annealing, vapor mixtures of toluene and n-heptane were used, which are weakly selective for PS and highly selective for PDMS, respectively. The morphological changes were investigated by in-situ, real-time grazing-incidence small-angle X-ray scattering (GISAXS). Varying the vapor composition during the annealing cycle results in a lamellar morphology and cylinders with different orientations. Using the scattering contrast, the distribution of the two solvents in the microphase separated thin film can be determined. This information can be transferred to a phase diagram and be related to the observed morphologies during annealing.

The results show that solvent exchange during SVA gives control over the morphology, and that GISAXS can be used to track the trajectory through the phase diagram experimentally.

CPP 49.3 Wed 18:30 P2-OG1

NPT Kinetic Monte Carlo Simulations of Photo-Switchable Molecules on a Surface — •Frederico Brückelmann, Matthew Dennison, and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Hardenberg Str. 36, 10623 Berlin, Germany

Photo-switchable molecules can undergo a light-induced trans-cis isomerization. Used as a functional group in polymers, one can fabricate porous media with light-switchable surface area, diffusivity, and permeability (e.g. for CO_2 and O_2 [1]). This promises new functional materials with reversible light-controlled macroscopic properties.

We use a molecular model for the porous medium, which builds on previous work in [2,3], where the trans and cis isomers are modeled as straight and bent hard-core needles, respectively. We develop a kinetic Monte Carlo simulation in the isothermal-isobaric ensemble that allows for moves in the system volume, which are coupled to the system's response time through the Frank elastic constants. We investigate the system's response as the molecules undergo trans-cis isomerization and monitore changes in volume and the distribution of pore sizes.

[1] D. Becker, N. Konnertz, M. Böhning, J. Schmidt, and A. Thomas, Chem. Mater. (2016), DOI:10.1021/acs.chemmater.6b02619.
[2] R. Tavarone, P. Charbonneau, and H. Stark, J. Chem. Phys. **143**, 114505 (2015).
[3] R. Tavarone, P. Charbonneau, and H. Stark, J. Chem. Phys. **144**, 104703 (2016).

CPP 49.4 Wed 18:30 P2-OG1

Adsorption Simulations of Plasma Proteins on Silica Surfaces — •Timo Schäfer[1,2], Giovanni Settanni[1,3], and Friederike Schmid[1] — [1]Johannes Gutenberg-University Mainz — [2]Graduate School Materials Science in Mainz — [3]Max Planck Graduate Center with the Johannes Gutenberg-University Mainz

Nanoparticle based therapeutics are a topic of ongoing research, promising effective use as drug delivery systems that shield aggressive and/or fragile drugs while transporting them to a target location inside the body. One of the major challenges in their application is the formation of a layer of adsorbed plasma proteins as soon as the nanoparticle enters the blood stream. This so-called protein corona can significantly impair the nanoparticle's functionality such as active targeting or enhancement of blood circulation times. While the corona formation can be limited, existing techniques cannot completely prevent it, and molecular details of the underlying mechanism are largely unknown. Here, we study the early adsorption of plasma proteins onto the surface of a silica nanoparticle using classical atomistic molecular dynamics simulations. Using a sophisticated silica surface model, adsorption dynamics, interaction patterns and the impact of the adsorption on protein structure and functionality are analyzed.

CPP 49.5 Wed 18:30 P2-OG1

Specific Ion Effects on the Adsorption and Structure of Dodecyl Sulfate Modified Air/Water Interfaces — Eric Weissenborn[1], •Christian Sauerbeck[2], and Björn Braunschweig[1] — [1]Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster, Germany — [2]Institute of Particle Technology (LFG), Friedrich-Alexander University of Erlangen-Nürnberg (FAU), Cauerstrasse 4, 91058 Erlangen, Germany

The influence of Li^+, Na^+ and Cs^+ cations on the coverage and structure of dodecyl sulfate (DS) anions at the air/water interface was investigated with a thin film pressure balance (TFPB) and vibrational sum-frequency generation (SFG). Particularly we have addressed the change in amplitude of O-H stretching bands which provides information on the charging state of the interface. That is because the static electric field within the interfacial's double layer can polar order and polarize interfacial H_2O molecules. As a consequence, the amplitude of O-H bands in SFG spectra becomes strongly dependent on the interfacial net charge. In addition, an analysis of the symmetric S-O stretching band at 1070 1/cm as a function of bulk salt and DS concentration provides information on the surface coverage and Gibbs free energies of adsorption when an adsorption isotherm is fitted to the experimental data. Here, we can show that the latter are a function of the bulk salt concentration and are ion specific. The magnitude of this ion specific effect decreases with the size of the alkali cation in the following way $Cs^+ > Na^+ > Li^+$.

CPP 49.6 Wed 18:30 P2-OG1

Stack of ultrathin Gallium layers — •Sebastian Runde, Heiko Ahrens, and Christiane A. Helm — Inst. of Physics, Greifswald University, D-17487 Greifswald

Fabrication of ultrathin conductive layers is important for many technological applications. We describe a forced wetting method for the formation of ca. 3 nm thin gallium layers that extent up to 10 cm^2. Optical and atomic force microscopy image the layers on different length scales. X-ray reflectivity measurements show that the Ga layers immediately form a sub-nm thick oxide coating at the film/air surface under ambient conditions. Different substrates are used successfully (Si wafers, partially oxidized Si wafers, borosilicate glass). Up to five layers can be formed by forced wetting on top of each other. According to X-ray reflectivity, the repeat distance of the Ga layers in the stack is 2.7-2.8 nm.

CPP 49.7 Wed 18:30 P2-OG1

Towards functionally graded latex films: preparation using plasma-electrochemistry during drying — Sebastian Hochstädt[1], Alexander Müller[1], •Heike Römermann[1], Oliver Höfft[2], Frank Endres[2], and Diethelm Johannsmann[1] — [1]Institute of Physical Chemistry, Clausthal University of Technology, Arnold-Sommerfeld-Str. 4, 38678 Clausthal-Zellerfeld — [2]Institute of Electrochemistry, Clausthal University of Technology, Arnold-Sommerfeld-Str. 6, 38678 Clausthal-Zellerfeld

Coatings with functionality varying from top to bottom have widespread applications. One way to achieve such gradients is surface treatment on dry films, for instance with a plasma or a flame. Here, we report on plasma treatment of wet films during drying. Both reductive and oxidative plasmas were used. In the first case, we employed a cold atmospheric argon plasma jet. The latex films contained metal salts, which, upon reduction, formed metal particles (copper and silver) on top of the film, or reduced potassium hexacyanoferrate (III) to change its color. These were studied with optical microscopy, SEM, and CLSM. Such particles can find applications as biocides. In the second case, an oxidative atmospheric DBD plasma was used to create a vertical gradient in the concentration of red potassium hexacyanoferrate (III) across the film. The salt had been introduced into the film in its yellow form and was oxidized to the red form. The gradient was qualitatively analyzed using UV-VIS spectroscopy and optical microscopy.

CPP 49.8 Wed 18:30 P2-OG1

Local dynamics in macromolecules at the interface to inorganic fillers — Jana Schaber[1], Franck Fayon[2], and •Ulrich Scheler[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V. — [2]CEMHTI CNRS Orleans

Dynamic NMR is well suited for the investigation of polymer chain dynamics. However NMR experiments are usually bulk measurements which yield an ensemble average. Two approaches are demonstrated for the selective excitation of protons from the polymer in the vicinity of the filler. A combination of T2 filter and chemical shift selection permits the selective excitation of the OH protons Hydroxyapatite nanoparticles. A second approach is based on heteronuclear magnetization transfer from the filler (29Si enriched silica) to the protons of the surrounding polymer. Subsequent spin diffusion transfers the magnetization further to the protons in the polymer matrix. A combination with relaxation experiments gives the relaxation time as a function of the distance to the filler particle. In the direct vicinity to the interface a shirt T2 indicative of restricted motion has been found. The combination with chemical shift resolution allows to attribute the observed relaxation times to functional groups or the water contained in the biomimetic nanoparticles.

CPP 49.9 Wed 18:30 P2-OG1

Direct photo alignment of tetracene via light-directed molecular self-assembly (LDSA) — •Linus Pithan[1,3], Paul Beyer[1], Laura Bogula[1], Anton Zykov[1], Peter Schäfer[1], Jonathan Rawle[2], Chris Nicklin[2], Andreas Opitz[1], and Stefan Kowarik[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik — [2]Diamond Light Source, Didcot, UK — [3]ESRF, Grenoble, France

There is an ongoing quest to tailor molecular thin film growth and thereby enhance the functionality of organic thin film structures. Here, we introduce light-directed molecular self-assembly (LDSA) to align and pattern molecular crystallites on amorphous, isotropic substrate.[1] We grow tetracene ($C_{18}H_{12}$) thin films on amorphous SiO_x surfaces via organic molecular beam deposition (OMBD) and study the direct-photo-alignment of molecular crystallites through 532 nm laser illumination, which matches the absorption band of the lower Davydov component of tetracene.

Based on LDSA we produce thin films that feature patterned, polarised optical emission due to the inherent anisotropic optical properties of aligned polycrystalline tetracene structures. We use grazing incidence X-ray diffraction (GIXD) as well as polarisation sensitive optical spectroscopy to analyse the degree of azimuthal alignment in the film and its dependency on the laser light intensity during growth.

[1] L. Pithan et. al. Adv. Mater. 2016 doi:10.1002/adma.201604382

CPP 49.10 Wed 18:30 P2-OG1

Sublimation enthalpy and vapor pressure of thermally instable substances from fast scanning calorimetry — •Amir Abdelaziz, Dzmitry Zaitsau, Sergey Verevkin, and Christoph Schick — University of Rostock, Germany

The determination of vapour pressure and corresponding enthalpy of sublimation lay within focus of many scientific fields and industrial applications. These values directly connected to the intermolecular forces in crystal state, provides the lattice energy and change in ordering by going from crystal to gas phase. In the present study the fast scanning calorimetry was successfully applied for determination of vapour pressure and enthalpies of sublimation of low volatile organic substances. In many cases investigation of such systems is accomplished with low thermal stability of them and application of classic techniques often fails by determining the decomposition rate of the system. The technique is based on the determination of the mass loss rate of the sample from the experimental total heat capacity and preliminary determined specific heat capacity of the compound under study. Sublimation of the sample is carried out during repeated isotherms of pre-defined duration and at selected temperatures. Sample is heated to needed temperatures at high heating rates accessible by this technique, what allows reaching the sublimation temperatures without any mass loss during the heating time. From the other side in the proposed technique the sublimation area is so big that sublimation mass loss rate is incomparably higher that decomposition rate. Thus the sample of tenth nano grams sublimes without any thermal degradation.

CPP 49.11 Wed 18:30 P2-OG1

Large-Area Surface Relief Gratings on Thin Films of Azobenzene-Containing Molecular Glasses — •Stefan Hartung[1], Lothar Kador[1], Andreas Schedl[2], Klaus Kreger[2], and Hans-Werner Schmidt[2] — [1]University of Bayreuth, Institute of Physics and BIMF, 95440 Bayreuth, Germany — [2]University of Bayreuth, Macromolecular Chemistry I, 95440 Bayreuth, Germany

Illumination of azobenzene-containing materials with a light intensity grating does not only give rise to a refractive-index modulation in the bulk but, depending on the type of material and the polarization state of the light, also to the formation of a surface relief grating (SRG). SRGs feature high diffraction efficiencies and are, therefore, promising candidates for technical applications such as diffractive optical elements (DOEs). We demonstrate that holographic illumination with two coherent expanded laser beams ($\lambda = 489$ nm) can efficiently produce SRGs with grating constant of 1 micrometer and diameter of more than 1 centimeter on thin films of an azobenzene-containing molecular glass. Due to the non-contact holographic generation, the gratings are virtually defect-free over the whole area. AFM measurements on various spots of the grating demonstrate that for short writing times, the amplitude follows the Gaussian cross section of the writing laser, whereas a more homogeneous amplitude distribution can be achieved with longer inscription. With laser powers of a few hundred milliwatts, typical writing times are on the order of several minutes. Repeated illumination under different rotation angles of the film gives rise to complex two-dimensional SRGs.

CPP 49.12 Wed 18:30 P2-OG1

Morphology improvement of ZnO/P3HT-b-PEO bulk heterojunction films by using a low temperature route — •Kun Wang[1], Yu Tong[2], Rui Wang[3], Stephan V.Roth[4], Lorenz Biessmann[1], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]LMU, Department für Physik und CeNS, Amalienstraße 54, 80799 München — [3]JCNS at MLZ, Lichtenbergstr. 1, 85748 Garching — [4]DESY, Notkestr. 85, 22607 Hamburg

Hybrid solar cells, a combination of conventional inorganic and organic photovoltaic systems, offer outstanding potential due to their minor investment compared to inorganic solar cells and higher stability compared to organic solar cells. However, so far device efficiencies are significantly lower as compared to the other photovoltaic systems. A possible way to improve the film structure and thereby the device efficiency is to introduce amphiphilic block copolymers into the sol-gel synthesis of the inorganic part such as ZnO. Unlike the traditional diblock copolymer, in the present approach we make use of a new functional block copolymer PEO-b-P3HT. In the PEO block the ZnO phase is synthesized and the P3HT block can be used directly as the hole transporting layer. The nanostructure inside thin films is probed with GISASXS. Moreover, SEM and AFM detect the surface morphology of the composite films.The optical properties are examined with UV/Vis spectroscopy and the thickness is investigated by profilometry measurements.

CPP 49.13 Wed 18:30 P2-OG1

Slip effects on forced dewetting — •Tak Shing Chan, Martin Brinkmann, and Ralf Seemann — Experimental Physics, Saarland University, D-66041 Saarbrücken, Germany

Slippage of fluid over a solid surface is known to have a weak (logarithmic) effect in macroscopic dynamic wetting. In this contribution, we study the forced dewetting of a liquid of viscosity η confined in a cylindrical tube of radius r_0 for a wide range of slip length b using the boundary element method. For $b \ll r_0$, the prediction of the critical velocity (U_c) of entrainment $Ca_c \equiv \eta U_c/\gamma \sim 1/\ln(cr_0/b)$ by classical dynamic wetting models is recovered. Here γ is the surface tension of liquid/air interface and c an undetermined prefactor. When increasing the slip length, we demonstrate a crossover from the logarithmic relation to a regime where Ca_c scales linearly with b for large b. In this regime, the energy input to the system is mainly dissipated by the friction at the solid/ liquid boundary. Our finding connects the dynamical wetting phenomena in macroscopic systems and small-scaled fluidic systems.

CPP 49.14 Wed 18:30 P2-OG1

Pinned and Sliding Drops – Bifurcations and Statistics — •Sebastian Engelnkemper, Markus Wilczek, Svetlana Gurevich, and Uwe Thiele — Institut für Theoretische Physik, Westfälische Wilhelms-Universität, Corrensstr. 2, 48149 Münster

The long-wave evolution equation for a liquid film (thin-film equation) describes the dynamics of free surface structures (e.g., drops and ridges) on solid substrates. On homogeneous substrates all structures move for any applied lateral driving force (e.g., inclining the substrate). They change their shape and may at a critical driving force undergo a pearling instability where large drops emit small satellite drops [1]. On heterogeneous substrates (e.g., with a wettability pattern) drops remain pinned at more wettable spots even at small driving force. At a critical driving the drops undergo a depinning transition as analyzed for 2d drops in [2]. Here we implement the thin-film equation in the continuation-toolbox PDE2PATH [3] and analyze shape changes of 3d sliding and pinned drops on homo- and heterogeneous substrates, respectively. Main control parameters are drop volume and substrate inclination. The pearling instability of sliding drops is identified as a global bifurcation of stationary sliding drops [4]. Finally, the single-drop continuation results are related to the drop size statistics obtained in direct simulations of large drop ensembles. [1] T. Podgorski et al., Phys. Rev. Lett. 87, 036102 (2001); [2] U. Thiele, et al., NJP 8, 313 (2006); [3] H. Uecker et al., arXiv:1208.3112v2 (2012); [4] S. Engelnkemper et al., Phys. Rev. Fluids 1, 073901 (2016);

CPP 49.15 Wed 18:30 P2-OG1

Utilizing Confocal Active Interference Scattering Microscopy to directly measure the phase of light scattered by a single nanoparticle — •Otto Hauler, Frank Wackenhut, Kai Braun, and Alfred J. Meixner — Institute of Physical and Theoretical Chemistry, Tübingen, Germany

In the recent years the optical properties of noble metal nanoparticles of different shapes and sizes have been widely studied and exploited by nanotechnology based assays. Especially gold nanoparticles are promising candidates for various applications due to their outstanding optical properties, which are dictated by their particle plasmons [1-4]. A powerful tool to investigate single gold nanoparticles is confocal scattering microscopy combined with higher order laser modes. We extended this established method in a way that allows us to directly measure the phase of the scattered light by introducing an interferometrical detection scheme similar to a Michelson interferometer. This enables us to measure the phase and amplitude of the light scattered by single gold nanoparticles and will enhance the usefulness of this imaging technique. [1] Frank Wackenhut, Antonio Virgilio Failla, Tina Züchner, Mathias Steiner, and Alfred J. Meixner, Applied Physics Letters 100 (26), 263102 (2012). [2] Frank Wackenhut, Antonio Virgilio Failla, and Alfred J. Meixner, The Journal of Physical Chemistry C 117 (34), 17870 (2013). [3] Frank Wackenhut, Antonio Virgilio Failla, and Alfred J. Meixner, Phys. Chem. Chem. Phys. 15 (15), 5407 (2013). [4] Frank Wackenhut, AntonioVirgilio Failla, and AlfredJ Meixner, Anal Bioanal Chem 407 (14), 4029 (2015).

CPP 49.16 Wed 18:30 P2-OG1

Silver iodide nanowires grown in amphiphilic tubular templates — •Egon Steeg, Katie Herman, Holm Kirmse, Jürgen P Rabe, and Stefan Kirstein — Institut für Physik, Humboldt-Universität zu Berlin

It was shown in previous work [1] that silver nanowires 6 nm in diameter can be grown by reduction of $AgNO_3$ in the presence of tubular aggregates of cyanine dyes in aqueous solution. Here we present an adaptation of this system for the growth of AgI structures by using additional iodide ions. Wire-like, single crystal structures of AgI that fill the inner space of the tubular aggregates are found. These AgI structures have diameters of 6 to 7 nm and lengths of tens of nanometers. The crystal structure of the AgI wires was investigated by means of high resolution transmission electron microscopy and selected area electron diffraction. The AgI could be clearly identified by its typical wurtzite structure. Small crystallites of pure silver can be found embedded in these AgI wires. The relative orientation of the respective crystal lattices indicates epitaxial growth of AgI on pure Ag or vice versa. It is possible that the negatively charged iodide ions have a higher concentration in the interior of the tubular aggregates than in the surrounding solution. This would favor the growth of AgI crystals within the tubules. These findings may demonstrate a possible route for growing other metal halide structures within the amphiphilic cyanine dye tubules.

[1] E. Steeg et al., Journal of Colloid and Interface Science 472(2016)187

CPP 50: Poster: Organic Electronics and Photovoltaics, Molecular Excitations

Time: Wednesday 18:30–21:00 Location: P3

CPP 50.1 Wed 18:30 P3

Solid state structure and charge transfer properties of D-A-D conjugated blocks: A joint experimental-theoretical approach — Deyan Raychev[1,2], Yevhen Karpov[1], Anton Kiriy[1], Jörg Grenzer[3], Jens-Uwe Sommer[1,2], and •Olga Guskova[1,2] — [1]Leibniz-Institute of Polymer Research Dresden, Hohe Str. 6 01069 Dresden — [2]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden — [3]Helmholtz-Zentrum Dresden-Rossendorf e. V., Bautzner Landstraße 400 01328 Dresden

The performance of molecular materials in organic electronics dramatically depends on their electronic properties and solid-state structure. In this work, we have investigated donor-acceptor-donor (D-A-D) conjugated molecules having central benzothiadiazole A-unit in order to understand the structure-property correlation by selecting thiophene or furan D-flanks. We have found, that the electronic and photophysical behavior is not affected, but the conformational and charge transfer properties exhibit a significant alteration upon varying a flank [1]. A joint theoretical packing prediction and experimental powder X-ray diffraction analysis showed differences in the solid-state structure and intermolecular interactions of D-A-D molecules. As a result, the difference in the solid-state packing defines the mobility of electrons and/or holes within the organic molecular stacks. The financial support from the ESF Group "CoSiMa" at DCMS, TU Dresden is highly appreciated.

[1] D. Raychev, O. Guskova, G. Seifert and J.-U. Sommer, Comp. Mater. Sci., 2017, 126, 287-298.

CPP 50.2 Wed 18:30 P3

Self-organization of liquid spread polymers for organic photovoltaics studied by 2d polarization microscopy — •Daniela Täuber[1], Wanzhu Cai[2], Olle Inganäs[2], and Ivan Scheblykin[1] — [1]Chemical Physics, Lund University, Lund, Sweden — [2]Biomolecular and Organic Electronics, Linköping University, Linköping, Sweden

Large-area self-assembly of functional conjugated polymers holds a great potential for practical applications of organic electronic devices. We obtain well aligned films of poly[2,3-bis(3-octyloxyphenyl)quinoxaline-5,8-diyl-alt-thiophene-2,5-diyl] (TQ1) by the floating film transfer method. Thereby, a droplet of a TQ1 solution is injected on top of the surface of a immiscible liquid substrate, at the meniscus formed at the edge of a Petri dish, from where the polymer solution and film then spreads in one direction. Characterization of the TQ1 film by the recently developed two-dimensional polarization imaging (2D POLIM) reveals large, mm sized domains of oriented polymer chains. The irregular shape of the contact line at the droplet source induced the appearance of disordered stripes perpendicular to the spreading direction. A correlation of polarization parameters measured by 2D POLIM revealed the microstructure of such stripes, providing valuable information for further improvement and possible upscaling of this promising method.

CPP 50.3 Wed 18:30 P3

Imidazo[1,5-a]pyridines as Light Emitting Materials — •Jasmin Martha Herr[1,3], Georg Albrecht[2,3], Julia Schulze[1], Derck Schlettwein[2,3], and Richard Göttlich[1,3] — [1]Justus-Liebig-University Giessen, Institute of Organic Chemistry — [2]Justus-Liebig-University Giessen, Institute of Applied Physics — [3]Justus-Liebig-University Giessen, Laboratory for Materials Science (LaMa)

Imidazo[1,5-a]pyridines display blue photoluminescence, tunable by introducing functional groups, and can be used as ligands to form coordination complexes. The goal of this work is the preparation and electro-optical characterization of imidazo[1,5-a]pyridine solutions and thin films as a prerequisite to their further investigation as stable blue-light emitting building blocks for OLEDs. We synthesized 1,3-disubstituted imidazo[1,5-a]pyridines with different substituents. The influence of these substituents on the electro-optical properties was measured in solution via UV-Vis spectroscopy, fluorescence spectroscopy and cyclic voltammetry as part of our research. For the application of imidazo[1,5-a]pyridines as emitting OLED building blocks, the electro-optical properties of the material in solid state have to be characterized. Therefore, we used spin-coating to fabricate thin films on different substrates and with different solvents.

CPP 50.4 Wed 18:30 P3

Thin Films of Imidazo[1,5-a]pyridines as Building Blocks of New Electro-Optic Devices — •Georg Albrecht[1,3], Jasmin Martha Herr[2,3], Frieder Müntze[1,3], Richard Göttlich[2,3], and Derck Schlettwein[1,3] — [1]Justus-Liebig-University Giessen, Institute of Applied Physics — [2]Justus-Liebig-University Giessen, Institute of Organic Chemistry — [3]Justus-Liebig-University Giessen, Laboratory for Materials Science (LaMa)

Imidazo[1,5-a]pyridines display blue photoluminescence, tunable by introducing functional groups, and can be used as ligands to form coordination complexes. The goal of this work is the preparation and electro-optical characterization of imidazo[1,5-a]pyridine thin films as a prerequisite to their further investigation as stable blue-light emitting building blocks for OLEDs. Suitable candidates for thin film preparation were chosen among 1,3-disubstituted imidazo[1,5-a]pyridines and deposited by spin-coating and physical vapor deposition. The optical absorbance of the samples was measured during film growth or subsequent to preparation by UV-Vis spectroscopy and morphological information was obtained by atomic force microscopy. The stability of samples was studied by storing the thin films either in the dark or under illumination and subsequent measurements of optical absorption. Cyclic voltammetry was used to obtain the redox potentials.

CPP 50.5 Wed 18:30 P3

Ultrafast Dynamics of Charge Transfer in Polymer-Fullerene Systems — •Stefan Wedler[1], Thomas Unger[1], Heinz Bässler[2], and Anna Köhler[1,2] — [1]Experimental Physics II, University of Bayreuth, 95440 Bayreuth, Germany — [2]Bayreuth Institute of Macromolecular Research (BAMF)

Exciton dissociation in organic semiconductors is a two-step process that consists first of an initial transfer of an electron from the photoexcited donor to the acceptor and second of the subsequent separation process of the resulting Coulomb-bound interfacial electron-hole pair. Here, we have explored whether the initial electron transfer is thermally activated and can thus be described by a Markus-type rate, or whether it is a temperature-independent tunneling-type process that is best modelled by a Miller-Abrahams rate. In order to investigate the influence of thermal activation on the transfer dynamics, we have performed temperature dependent ultrafast pump-probe spectroscopy on films of three polymer-PCBM blends with a resolution of 200 fs. The charge transfer is measured by monitoring the transient absorption of the polymer cation after excitation. So far we find no change in transfer dynamics upon cooling to low temperatures within our temporal resolution. This result suggests that initial charge transfer lacks thermal activation.

CPP 50.6 Wed 18:30 P3

Investigation of ZnO scattering layers for OLED applications — •Dominik Schullerer, Lorenz Biessmann, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Organic light emitting diodes (OLED) are reaching inner quantum efficiencies close to 100%, but the overall efficiency of conventional devices is limited to about 20% mainly by the photon extraction. One approach to overcome this issue is the implementation of an additional scattering layer into the device. A standard OLED is used to study the impact of such layer. This layer can either be created by a direct surface structuring or the introduction of an additional transparent layer. Zno is a suitable choice for the latter due to its transmittivity in the entire visible spectrum, caused by its direct optical bandgap of 3.3eV. This layer is deposited on a glass substrate. The micro- and nano-structure of ZnO can be adjusted by combining a structure-giving diblock copolymer with sol-gel chemistry. It is investigated how different structuring, which is analyzed by scattering techniques and electron microscopy, can influence the external quantum efficiency and the macroscopic properties of the OLEDs over the entire spectral range.

CPP 50.7 Wed 18:30 P3

Investigation of an n-type conducting polymer for potential use in all-polymer thermoelectric generators — •Regina Michaela Kluge, Nitin Saxena, and Peter Müller-Buschbaum — Technische Universität München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Thermoelectric generators pose a promising approach in renewable energies, as they are able to convert waste heat into electricity. In order to build high efficiency devices, suitable thermoelectric materials are needed. Unfortunately, state-of-the-art thermoelectric materials have the drawback of using toxic or less abundant constituents, making it necessary to look for alternatives. One promising approach is to use conjugated polymers. They have the encouraging ability of easy and various types of scalable solvent processes like roll-to-roll printing. Although they are still less efficient than their inorganic counterparts, their easy synthesis, flexibility and eco-friendliness make them a valuable alternative. For building a thermoelectric generator, p- and n-type materials have to be combined. However, in the past effort was focused on the electronic and thermal transport properties of p-type conjugated polymers. Therefore, we investigate the thermoelectric properties of an n-type polymer P(NDI2OD-T2). Its successful application to transistors and solar cells encourages an auspicious try to build an all-polymer thermoelectric generator.

CPP 50.8 Wed 18:30 P3

Solvent Induced Galvanoluminescence of Metal-Organic Framework Electroluminescent Diodes — •Haonan Huang[1], Michelle Beuchel[2], Dago de Leeuw[2], and Kamal Asadi[2] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart — [2]Max Planck Institute for Polymer Research, D-55128 Mainz

Alternating current (AC) electroluminescent diodes were fabricated from MOF-5, a metal organic framework consisting of tetrahedral $[Zn_4O]^{6+}$ units linked by 1,4-benzenedicarboxylate ligands. An additional insulating layer was incorporated to prevent formation of electrical shorts. The electroluminescence spectrum was dramatically redshifted with respect to the photoluminescence spectrum. By deliberately varying trapped solvent molecules, we demonstrate that the light emission does not originate from MOF-5 but is due to galvanoluminescence, emission of weak optical radiation in the visible region that occurs during anodic oxidation of the Al top electrode in contact with electrolytes.

CPP 50.9 Wed 18:30 P3

Comparison of theoretical and actual benefit of birefrigent layers in OLEDs — •Markus Schmid, Thomas Lampe, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

One of the main factors influencing the efficiency of OLEDs is the microcavity formed by the organic layers enclosed between the electrodes. From a theoretical point of view it was shown that the inclusion of a birefrigent material as transport layer at the reflective cathode can improve the outcoupling efficiency of such devices [1]. The main reason for this is reduced coupling to surface plasmons at the organic-metal interface due to the effects of the anisotropic material.

In this work we present an OLED-layout using a birefrigent electron transport layer and a reference device with isotropic optical constants. However, the main challenge is that most optically anisotropic organics like TCTA or Spiro-2CBP are hole-conductors not suitable for electron-transport. Additionally the use of electron injection layers would prevent the beneficial effects of the anisotropic material. In order to reach the necessary electric properties we doped the organic material. Making use of electrical and optical simulations as well as a heteroleptic phosphorescent emitter, we achieved a highly efficient OLED with a birefrigent layer in contact to the reflective cathode. The devices even show an external quantum efficiency close to their theoretical limit of about 21 %.

[1] Callens, Michiel K. et al.: Anisotropic materials in OLEDs for high outcoupling efficiency. *Optics express* 23, p.21128–21148 (2015).

CPP 50.10 Wed 18:30 P3

Molecular Dynamics Simulations of Perylene Bisimide Dimers — •Sebastian Johannes Müller, Axel Bourdick, and Stephan Gekle — Universität Bayreuth

Investigating the stacking mechanism of two perylene bisimide dimers by means of free energy calculations with the molecular dynamics implementation Gromacs shall explain the great difference in their suitability for organic solar cells. The dimers consist of two perylene molecules linked by a short alkane chain whose length differs by one carbon atom. We clarify how different configurations in the stacked state affect the π-π-stacking ability and further show that the dimer with the longer link gains more free energy during a stacking process and has more stable stacked states and configurations than the other.

CPP 50.11 Wed 18:30 P3

Proton Beam Writing in Alq3 — •Clemens Beckmann, Alrik Stegmaier, Ulrich Vetter, and Hans Hofsäss — II. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Proton Beam Writing (PBW) is a direct-write lithography process for nano- and microfabrication of two- or three-dimensional structures [1]. The straight path and low proximity effect of MeV protons in matter allow for the fabrication of structures with high aspect ratio and vertical smooth sidewalls. PBW has been widely studied in resists for lithography and conventional semiconductors like Si and GaAs [1,2]. In this work we focus on PBW in organic semiconductors, which are the key materials in the fast growing field of organic optoelectronics. We will discuss possible ways for structuring of tris(8-hydroxyquinoline)aluminum (Alq3) and present experimental results on the irradiation of Alq3 thin films with high energy protons.

[1] Watt et al, Materials Today 10 6 (2007)

[2] Schulte-Borchers et al, J. Micromech. Microeng. 22 (2012)

CPP 50.12 Wed 18:30 P3

Influencing emitter orientation in solution processed guest-host-sytems — •Philippe Linsmayer, Thomas Lampe, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

The beneficial horizontal alignment of the transition dipole moments in heteroleptic Ir-complexes is dominated by the interaction at the aromatic film surface during the step-by-step layer deposition in thermally evaporated films. In order to probe weaker molecular interactions besides these effects, we studied phosphor alignment in solution processed guest-host systems. While this approach is not giving the possibility for horizontal alignment of the transition dipole moments, it reveals the influence of the processing parameters like dopant concentration, glass-transition temperature of the host and impact of thermal annealing in solution processed films. For the experiments a common heteroleptic Ir-complex was doped into four different host materials with varying glass transition temperatures. After deposition the films were treated with thermal annealing near the glass transition temperature. The results indicate dependence of the resultant emitter orientation on several parameters which can be attributed to different molecular interactions inside the guest-host system.

CPP 50.13 Wed 18:30 P3

controlling excitons in exciplex host systems for efficient white OLEDs — •Yuan Liu, Simone Lenk, Karl Leo, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, George-Bähr-Straße 1, 01069 Dresden, Germany

White organic light-emitting diodes (WOLEDs) are highly attractive for flexible displays and lighting panels due to their ultrathin form factor, low cost, good color quality, and high power efficiency. Here, an exciplex system consisting of mCP and B3PYMPM is demonstrated to achieve high efficiency blue and white OLEDs. Employing Iridium(III) bis[(4,6-difluorophenyl)pyridinato-N, C2*] picolinate (FIrpic) as emitter, an external quantum efficiency (EQE) of 19.1% is realized by optimizing the hole and electron transporting layer. Triplet-triplet annihilation and triplet-polaron quenching models are utilized to understand the efficiency roll-off of the devices. Based on optimized blue OLEDs, an efficient WOLED with maximum 19.5% EQE (50.6 lm/W) has been realized by carefully controlling exciton generation and transfer processes. At the practical brightness of 1000 cd/m2, it still keeps 18.8% EQE (42.7 lm/W). Adopting a glass half sphere as a light outcoupling technology, the luminous efficacy of the WOLED reaches a maximum of 84.9 lm/W with Commission International de L*Eclairage coordinates of (0.452, 0.457) and a color rendering index of 81. Further, the influence factors of color stability and efficiency roll-off in exciplex-based WOLEDs are investigated in detail.

CPP 50.14 Wed 18:30 P3

Efficient Deep-blue Pyridimidine-based TADF Emitters Using a Highly Twisted Molecular Skeleton — •Ryutaro Komatsu[1], Tatsuya Ohsawa[2], Hisahiro Sasabe[1,2,3], Kohei Nakao[1], Yuya Hayasaka[1], and Junji Kido[1,2,3,4] — [1]Department of Organic Materials Sience, — [2]Faculty of Engineering, — [3]Research Center for Organic Electronics (ROEL), — [4]Frontier Center for Organic Materials (FROM), Yamagata University, 4-3-16 Jonan, Yonezawa, Yamagata, 992-8510, Japan

The development of efficient deep-blue emitters is one of the key issues in organic light-emitting devices (OLEDs). As a promising technology that realizes 100% conversion from electrons to photons, thermally activated delayed fluorescence (TADF) emitters have attracted considerable attention. However, only a few efficient deep-blue TADF emitters have been reported to date. Here, we molecularly manipulated the electronic excited state energies of pyrimidine-based TADF emitters to realize deep-blue emission. We then systematically investigate the relationships among the chemical structure and optical properties. The resultant novel pyrimidine emitters called Ac-XMHPMs (X = 1, 2, and 3) contain different numbers of bulky methyl substituents at acceptor moieties, increasing the excited singlet and triplet state energies. Among them, Ac-3MHPM, with a high triplet state energy of 2.95 eV exhibits a high peak external quantum efficiency (EQE) of 18% and an EQE of 10% at 100 cd/m2 with Commission Internationale de l'Eclairage chromaticity coordinates of (0.16, 0.15). These efficiencies are among the highest values to date for deep-blue TADF-OLEDs.

CPP 50.15 Wed 18:30 P3

Influence of sidechains on the aggregation behavior of polythiophenes — •Konstantin Schötz[1], Tobias Meier[1], Dominic Raithel[2], Daniel Schiefer[3], Michael Sommer[3], Fabian Panzer[1], Richard Hildner[2], and Anna Köhler[1] — [1]Experimental Physics II, Universität Bayreuth — [2]Experimental Physics IV, Universität Bayreuth — [3]Department for Macromolecular Chemistry, Albert-Ludwigs-Universität Freiburg

Polythiophenes are known to often undergo a phase transition from a high energy coiled phase to a low energy aggregated phase upon cooling or spin coating. The properties of these aggregates have strong impact on the performance of devices like OFETs or solar-cells. It is known that these properties and the characteristics of the aggregate formation depend on different parameters like chain length, polydispersity or concentration of the solution. We measured temperature dependent absorption and emission on various polythiophenes that differ in their sidechain architecture. We show that the electronic structure and thus the character of the formed aggregates depend strongly on the type of the sidechains.

CPP 50.16 Wed 18:30 P3

Thermally Activated Delayed Fluorescence studied by Electroluminescence Detected Magnetic Resonance — •Sebastian Weissenseel[1], Nikolai Bunzmann[1], Benjamin Krugmann[1], Jeannine Grüne[1], Stefan Väth[1], Andreas Sperlich[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg

The mechanism of thermally activated delayed fluorescence (TADF) in organic light emitting diodes (OLEDs) raised many questions with respect to the spins of the emitting exciplex states. In particular, whether the TADF mechanism is a spin-dependent process and, if yes, what is the mechanism of the triplet-singlet Up to now spin-sensitive measurements for OLED devices are scarcely presented in literature. Here, we investigate TADF OLEDs by electroluminescence detected magnetic resonance (EL-DMR) in devices based on 4,4',4"-Tris(N-3-methylphenyl-N-phenylamino)triphenylamine (m-MTDATA): Tris(2,4,6-trimethyl-3-(pyridin-3-yl)phenyl)borane (3TPYMB) exciplexes. The triplet states of this system energetically split in an external magnetic field. Microwave radiation, applied by a stripline, is absorbed at a resonant magnetic field and enhances the intensity of electroluminescence. Modifying experimental conditions, e.g. resonance frequency, temperature or microwave power, leads to detailed knowledge of the spin system and the underlying mechanism of the reverse intersystem crossing. This information will assist designing new cost-effective OLED materials.

CPP 50.17 Wed 18:30 P3

Towards high-mobility polymorphs in organic semiconductors — •Daniel R. Reiterer, Simon Erker, Egbert Zojer, and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

An important aspect for the application of organic semiconductors in practical devices is their charge-carrier mobility. However, in organic molecules the mobilities are often small. One of the reasons is that organic molecules tend to crystallize in polymorphs with a small band dispersion and that polymorphs with large dispersion tend to be energetically unfavorable. This is because increasing the intermolecular wave-function overlap, which would increase the band dispersion, also increases Pauli-repulsion. In this work, we discuss various strategies to mitigate or circumvent this effect in order to achieve high-mobility (high dispersion) polymorphs of organic semiconductors. For the example of pentacene we show that high-dispersion polymorphs can be stabilized when the antibonding states in the valence band are depleted. This can be achieved via doping or, to a lesser extent, via contact with passivated metal surfaces. Another possible strategy that we demonstrate here is the use of antiaromatic molecules such as cyclooctatetraene (COT).

CPP 50.18 Wed 18:30 P3

Degradation in polymer-fullerene bulk heterojunction solar cells due to charge carrier recombination — •Eliuter Nderimo, Arne Müller, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Organic solar cells have become an increasingly important form of solar cells in recent years. The prolonged illumination of solar cells under sunlight usually leads to a slow reduction of their efficiency. Studying their degradation allows us to accurately predict their power delivery over time. In this work we will focus on the recombination dynamics of PTB7:PCBM bulk-hetero junction solar cells under prolonged illumination. We show that the change in efficiency of the solar cells over time due to charge carrier recombination is a dominating factor of degradation. This is done by applying different potential biases to the cell under continuous AM1.5G equivalent illumination. The lifetime of the solar cell is decreased by a factor of 10 if the charges recombine in the semiconductor bulk (Voc condition) instead of being extracted (Jsc condition). Other means of degradation, such as oxygen and water vapour interference, were minimized by encapsulation. From dark measurements the pure degradation by recombination is extracted and supports the observed effect under illumination.

CPP 50.19 Wed 18:30 P3

Synthesis and characterisation of the new emitters for OLED applications — •Ramunas Lygaitis[1,2], Olaf Zeika[1], Reinhard Scholz[1], Ludwig Popp[1], Paul Kleine[1], Simone Lenk[1], and Sebastian Reineke[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Deutchland — [2]Kaunas University of Technology, Kaunas, Lithuania

Organic light-emitting diodes (OLEDs) are a sustainable, low cost light source used in displays and other applications. Quite big step in progress was made when phosphorescent materials containing Ir(III), Pt(III), or other heavy metals were used in order to harvest both singlet and triplet excitons by means of enhanced intersystem crossing. Today, one of the issues which prevent current iridium-based, phosphorescent emitters widely used in the lighting markets, is that iridium is the fourth rarest naturally-occurring element on the planet, so the usage of this element in large scales could be very risky. Therefore new iridium-free emitters harvesting both singlet and triplet excitons are of big interest. Here, we present the synthesis and characterisation of the series of carbazole-based derivatives containing electron accepting trifluoromethyl groups which support certain intermolecular charge transfer. The newly synthesised derivatives were characterised by means of absorption spectroscopy, steady-state and time-resolved fluorescence spectroscopy, and cyclic voltametry. The collected data prove that our new materials could be regarded as potential TADF emitters as well OLEDs have been prepared with reasonable efficiencies.

CPP 50.20 Wed 18:30 P3

Tuning organic solar cells via doping with inorganic nanoparticles — •Sebastian Grott, Nuri Hohn, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Organic solar cells have attracted increased attention due to their advantages in tunable characteristics, low-cost manufacturing processes and flexibility, which opens up a promising alternative for conventional photovoltaics. Recently the most widely investigated bulk heterojunction donor-acceptor system of P3HT:PCBM was doped with iron oxide nanoparticles, resulting in an increase of efficiency.[1] Based on this approach, we investigate the effect of doping P3HT:PCBM active layers with alternative inorganic nanoparticles. We study the influence of different inorganic nanoparticle concentrations on current density-voltage characteristics and the absorbance. These optoelectronic properties are compared with structure information deteremined with scattering methods. [1] D. M. González, V. Körstgens, Y. Yao, L. Song, G. Santoro, S. V. Roth, P. Müller-Buschbaum, Adv. Energy Mater. 2015, 5, 1401770.

CPP 50.21 Wed 18:30 P3

Investigation of Spin States Involved in Thermally Activated Delayed Fluorescence by Magnetic Resonance Methods — •Benjamin Krugmann[1], Nikolai Bunzmann[1], Sebastian Weissenseel[1], Jeannine Grüne[1], Andreas Sperlich[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg

Organic light emitting diodes (OLEDs) based on thermally activated delayed flourescence (TADF) can exhibit a maximum internal quantum efficiency (IQE) of 100% instead of the 25% IQE that classical fluorescence emitters reach. The TADF mechanism is believed to include thermally induced reverse intersystem crossing (RISC) between slightly energetically split triplet and singlet states of exiplexes. Here, we present measurements based on bilayer 4,4',4''-Tris[phenyl(m-tolyl)amino]triphenylamine:Tris(2,4,6-triMethyl-3-(pyridin-3-yl)phenyl)borane (m-MTDATA:3TPYMB) OLEDs. We are using the spin sensitive method of electroluminescence detected magnetic resonance (ELDMR), in which spin states are energetically separated by an external magnetic field. Additionally, we apply microwaves to excite transitions between triplet states at resonance, where the emission of electroluminescence is elevated. By investigation of the resonant peak at different parameters we can draw conclusions about the spin dependent mechanisms involved in the TADF process.

CPP 50.22 Wed 18:30 P3

Charge carrier dynamics in bilayer coupled organic-inorganic nanostructures — •Florian Grassl[1], Alexander Hofmann[1], Eduard Meister[1], Alexander André[2], Michelle Weber[2], Marcus Scheele[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Institute for Physical and Theoretical Chemistry, University of Tübingen, 72076 Tübingen, Germany

Coupled organic-inorganic nanostructures (COINS) utilize organic semiconductors as crosslinking ligands to facilitate charge conduction between semiconductor nanocrystals. They offer the perspective to combine efficient carrier transport with a high degree of structural order [1], as it has been successfully demonstrated in field-effect transistors [2]. Here we focus on out-of-plane charge carrier dynamics of COIN layers in diodes and solar-cells. Using three different techniques of fabricating COIN layers from PbS nanocrystals with Cu-phthalocyanine as organic linker molecules, we elucidate the influence of preparation conditions on carrier transport and device performance. Additionally we compare different organic and inorganic hole injection layers and the impact of the COIN production process on their electrical properties.

[1] M.Scheele *et.al.*, Physical Chemistry Chemical Physics (2015), doi:10.1039/c4cp03094j
[2] A.André *et al.*, Chemistry of Materials (2015), doi:10.1021/acs.chem mater.5b03821

CPP 50.23 Wed 18:30 P3

Structuring of insoluble polythiophene for organic solar cells — •Eva Maria Kratzer, Jenny Lebert, and Eva Maria Herzig — TU München, Munich School of Engineering, Herzig Group, 85748 Garching

Polythiophene, an insoluble semiconducting material, can be used as donor material in organic polymer solar cells. However, to cheaply process this material from solution the insolubility needs to be taken into account. Therefore, it is synthesized *in situ* from the soluble monomer to make it processable in solution. Advantages of the polythiophene are the low costs and the high availability of the used material for the synthesis. An important property for organic solar cells fabrication is a high degree of interfacial control between the donor and acceptor material for efficient charge separation.

In this work, we exploit the insolubility of the polythiophene thin films for processing of structured multilayers. Different approaches are shown to achieve well-defined, structured donor-acceptor interfaces. The structured multilayers are investigated regarding their geometric from on various length scales and the resulting influence on the electronic properties is systematically analyzed with microscopy, spectroscopy and scattering.

CPP 50.24 Wed 18:30 P3

Hybrid quantum dots: poly(3-hexylthiophene) solar cells — •Wei Chen[1,2] and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]Department of Electrical and Electronic Engineering, Southern University of Science and Technology, 518055 Shenzhen, China

Blends of semiconducting polymers and inorganic semiconductor nanocrystals, like quantum dots (QDs), have started to attract intensive interests because of their inexpensive costs and the abilitiy of being solution processed. Both facts render them very promising candidates for next generation organic photovoltaics. Hybrid bulk heterojunction (BHJ) solar cells integrated with CuInSexS2-x (CISS) QDs and poly(3-hexylthiophene) (P3HT) are under investigation. CISS QDs are used as acceptor in our BHJ solar cell schematic, due to their strong optical absorption, tunable band-gap reaching to near infrared and long exciton lifetime, while P3HT is employed as donor material. The surface engineering of the QDs is investigated as a key factor to increase the exciton diffusion length and therefore improve the performance of solar cell devices. The QDs- P3HT active layers with 120 nm thickness are fabricated by blending using the spin-coating method. Different blend ratios are compared.

CPP 50.25 Wed 18:30 P3

Coupling of organic light emitting diode emission to planar waveguides — •Toni Bärschneider[1], Simonas Krotkus[2], Simone Lenk[1], Sebastian Reinecke[1], and Karl Leo[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, Germany — [2]School of Physics and Astronomy, St Andrews, United Kingdom

Organic light-emitting diodes (OLEDs) are cheap, bright, and easy-to-fabricate light sources which can be deposited on arbitrary substrates. For these reasons, successful OLED integration on the planar waveguide structure is advantageous for a wide range of applications, including point-of-care sensing and optical circuits. However, due to the optical absorption of the electrodes, efficient coupling of OLED emission into the thin waveguide core lying beneath is one of the major challenges. One promising approach is to make use of evanescent coupling, which relies on the overlap between emission and waveguide mode. However, there are number of possible improvements in efficiency and composition of light. Here especially, one targets blue light emission for compatibility with common analytes as well as light that is TM polarized. In this work, we investigate the waveguide coupling of a blue OLED to a 70 nm TiO$_2$ layer. A p-i-n device design enables optical optimization guided by numerical calculations, while the use of the thin metal electrode is shown to be beneficial for an efficient light incoupling. A highly transparent, easy and effective ALD encapsulation is used to carry out measurements under ambient conditions.

CPP 50.26 Wed 18:30 P3

Investigations on Band Structure Engineering in Organic Semiconductors — •Katrin Ortstein[1], Martin Schwarze[1], and Karl Leo[1,2] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials, TU Dresden, Germany — [2]Fellow of the Canadian Institute for Advanced Research, Toronto (ON), Canada

In modern electronics, it is essential to create almost arbitrary band structures by adjusting the energy bands and the band gap. Until now, a possibility of band structure engineering in organic semiconductors has not been possible, since they usually exhibit localized electronic states instead of energy bands. In a recent publication [1], we showed that it is possible to continuously shift the ionization energy of organic semiconductors over a wide range by mixing them with halogenated derivatives. This tuning mechanism is based on long-range interactions of excess charges with the mean quadrupole field in the thin film.

In this work, we further investigate this phenomenon using ultraviolet photoelectron spectroscopy measurements and set the focus on the range of these charge-quadrupole interactions. For this purpose, we study blended layers composed of C$_{60}$, ZnPc and F$_8$ZnPc and additionally probe stepwise the electronic levels at their flat interfaces.

[1] Schwarze et al., Science 352, 1446 (2016)

CPP 50.27 Wed 18:30 P3

A Novel Approach to Align Small Molecules Thin Films by Light-Directed Molecular Self-Assembly — •Andika Asyuda, Linus Pithan, Anton Zykov, Andreas Opitz, and Stefan Kowarik — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Germany

For the functionality of organic thin film devices, several film's structural properties, such as surface morphology, polymorphism, and molecular alignment, are known to be highly important. Recently light-directed molecular self-assembly (LDSA) was shown to promote a growth of aligned tetracene film(1). The versatility of this technique motivates us to closely investigate various related aspects, such as its implication on transport properties due to an optimization in molecular alignment. In this contribution we presented the state of art of LDSA toward a realisation of organic transistor with an increased mobility, due to an enhanced crystallinity and anisotropy in a molecular thin film.

1. L. Pithan, P. Beyer, L. Bogula, A. Zykov, P. Schäfer, J. Rawle, C. Nicklin, A. Opitz,and S. Kowarik, Adv. Mater. 2017 , 1604382

CPP 50.28 Wed 18:30 P3

Fabrication of organic nanowires by melt infiltration of a discotic liquid crystal: A combined X-ray diffraction and optical birefringence study — •Kathrin Sentker[1], Arda Yildirim[2], Andreas Schönhals[2], and Patrick Huber[1] — [1]Institut für Werkstoffphysik und -technologie, Technische Universität Hamburg-Harburg — [2]Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin

Discotic liquid crystals (DLC) can exhibit a liquid crystalline phase with their molecules oriented along one specific direction forming hexagonal arranged columns. Embedded in nanoporous membranes the columns orient perpendicular (radially) or parallel (axially) with respect to the pore axis. Due to their hydrophilic nature porous membranes enforce face-on anchoring leading to a radial orientation. Axially oriented columns ensure high conductivity in the stacking direction due to overlapping pi - electrons yielding interesting applications in e.g. organic semiconductor-based devices. Optical birefringence measurements show that we successfully realized an axial orientation by embedding the DLC HAT6 in an alumina membrane with a pore size of 25 nm. We suspect that anions introduced into the membrane lattice from the manufacturing process react with the DLCs changing the anchoring condition of the membrane. This enforces edge-on-orientation leading to an axial orientation of columns. XRD experiments giving detailed information about the translational order support the findings from optical measurements.

CPP 50.29 Wed 18:30 P3

Measuring C60 diffusion in the low bandgap copolymer PCDTBT — •Denys Priadko[1], Thomas Müller[1], Christina Saller[2], Tobias Hahn[1], Julian Kahle[1], Steffen Tscheuschner[1], Peter Strohriegl[2,3], and Anna Köhler[1,3] — [1]Experimental Physics II, University of Bayreuth, 95440, Bayreuth, Germany — [2]Macromolecular Chemistry I, University of Bayreuth, 95440, Germany — [3]Bayreuth Institute of Macromolecular Science (BIMF), University of Bayreuth, 95440, Bayreuth, Germany

Although diffusion of fullerenes in blend or bilayer heterostructures has a strong impact on the efficiency and long-term stability of organic solar cells and other organic electronic devices, little is known about the diffusion coefficient of fullerenes in different materials. We have recently shown that the C60 diffusion in the high bandgap homopolymer polyfluorene can be reduced by a factor of 1000 by crosslinking the polymer. We have now extended our approach to the low bandgap copolymer PCDTBT. We study how crosslinking PCDTBT suppresses the diffusion of C60 into it compared to inserting a LiF layer between the PCDTBT and the C60.

CPP 50.30 Wed 18:30 P3

Charge stability on polypropylene electrets with surfaces treated in orthophosphoric acid — •Jingwen Wang and Dmitry Rychkov — University of Potsdam, Potsdam, Germany

It is known that both, physico-chemical surface modification and thermal treatment, can lead to enhanced electret properties of dielectric polymers. To further investigate the influence of surface modifications on charge storage in polypropylene (PP) electrets, a combined thermal and chemical treatment with orthophosphoric acid (H3PO4) is applied to PP films. Charged samples are then studied by means of thermally-stimulated discharge (TSD) experiments, contact-angle measurements and Fourier-transform infrared (FTIR) spectroscopy. From the results, it can be concluded that additional deeper traps have been formed along with the treatment-induced conformation variations on the surface of the PP films. The new traps significantly improve the surface charge-stability of PP electrets.

CPP 50.31 Wed 18:30 P3

Fluorescence Lifetime Imaging Microscopy on Different Samples of the Conjugated Polymer P3HT — •Viktor Messerer[1], Lothar Kador[1], Richard Hildner[2], Hannes Welz[3], and Hans-Werner Schmidt[3] — [1]University of Bayreuth, Institute of Physics and BIMF, 95440 Bayreuth, Germany — [2]University of Bayreuth, Experimental Physics IV, 95440 Bayreuth, Germany — [3]University of Bayreuth, Macromolecular Chemistry I, 95440 Bayreuth, Germany

A custom-built fluorescence lifetime imaging microscope operating in the frequency domain (FD-FLIM) was used for mapping the fluorescence lifetimes of different samples of the conjugated polymer poly(3-hexylthiophene) (P3HT). Excitation was performed with a diode laser ($\lambda = 488$ nm) amplitude-modulated at frequencies between 104 and 160 MHz. Thin films of P3HT which contain a small amount of a tailored supramolecular nucleating agent to allow for the formation of highly ordered P3HT nanofibers were investigated. Neat P3HT was used as a reference. The fluorescence lifetime is obtained from the modulation amplitude of the fluorescence and its phase shift with respect to the excitation. The measured lifetimes are distinctly below 100 ps with the longest values found in the vicinity of the nucleating fibers. This result is ascribed to improved order of the H-aggregated P3HT nanofibers.

CPP 50.32 Wed 18:30 P3

In-situ polymerized PEDOT: Tos thin films for thermoelectric applications — •Mubashar Rafiq, Nitin Saxena, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Thermoelectric materials are an efficient tool to convert waste heat into electrical energy in an environment-friendly manner. These materials make use of the Seebeck effect for the transformation of heat into electrical energy. PEDOT: TOS thin films show higher Seebeck coefficients and conductivities as compared to PEDOT: PSS, and these quantities play a key role for the figure of merit ZT. To improve these quantities an in-situ polymerized PEDOT: TOS is studied with respect to adding additives and performing pre- and- post- treatments of thin films with different chemicals. Measurements of above mentioned quantities are carried out by four probe method and thermo voltage setup. Moreover, we are trying to deduce how these quantities could be affected by polymerization, polymer chain length, morphology, crystallinity and structural changes. For this purpose we use UV-Vis, AFM and x-ray scattering methods.

CPP 50.33 Wed 18:30 P3

Substrate Influence on the Formation of 2D-Polymeric Phthalocyanine Sheets — •Clemens Geis[1,2], Thi Hai-Quyen Nguyen[1,2], Pascal Schweitzer[1,2], and Derck Schlettwein[1,2] — [1]Justus-Liebig-University Giessen, Institute of Applied Physics — [2]Justus-Liebig-University Giessen, Laboratory for Materials Science (LaMa)

Phthalocyanines can be synthesized as two-dimensional polymeric sheets. Interest in their electrical properties and, e.g., in their use as electrode materials in catalysis is rising. Compared to monomeric phthalocyanines, the sheet polymers are characterized by an enhanced mechanical and chemical stability. The synthesis of those networks critically depends on the control of various reaction parameters. This work focuses on the influence of the substrate during a two-step reaction of 1,2,4,5-tetracyanobenzene with copper under vacuum conditions. Diffusion effects, side reactions and alloying within the substrate can hinder or even disrupt the formation of the phthalocyanine network and, hence, lead to undesired results. Spectroscopic methods were used to define and control the influence of the substrate on the growth of the 2D phthalocyanine network.

CPP 50.34 Wed 18:30 P3

Current-Voltage Characteristics of Polymeric Phthalocyanine Thin Films — •Thi Hai Quyen Nguyen[1,2], Clemens Geis[1,2], and Derck Schlettwein[1,2] — [1]Justus-Liebig-University Giessen, Institute of Applied Physics — [2]Justus-Liebig-University Giessen, Laboratory for Materials Science (LaMa)

Polymeric phthalocyanines as organic semiconductors have shown a wide range of electrical conductivity. In this work, polymeric copper phthalocyanine (CupPc) thin films were prepared by a reaction of tetracyanobenzene (TCB) with thin copper films on insulating substrates. In order to allow electrical measurements in a two-point-probe geometry electrodes of Au or Ni were vapor-deposited either directly on the substrate before film preparation or onto the prepared film subsequent to its growth. Conductivities of the organic films were determined from the current-voltage curves. The film thickness was measured with the help of a confocal laser scanning microscope and a scanning electron microscope. A more detailed examination of the cross-section of the samples revealed that either sponge-like or compact films could be formed dependent on the reaction temperature. Excess metallic copper remaining in the films after the reaction showed a strong influence on the electrical measurements as seen by thorough variation of the copper film thickness. Using X-ray diffraction the existence of metallic copper in the sample was analyzed and the presence of polymeric phthalocyanines was clearly validated.

CPP 50.35 Wed 18:30 P3

Development of a Procedure for the Synthesis of Two-Dimensional Polymeric Phthalocyanines Under High Vacuum Conditions — •Pascal Schweitzer[1,2], Clemens Geis[1,2], and Derck Schlettwein[1,2] — [1]Justus-Liebig-University Giessen, Institute of Applied Physics — [2]Justus-Liebig-University Giessen, Laboratory for Materials Science (LaMa)

As two-dimensional polymeric structures are of special interest in current research and phthalocyanine-based molecules can be used in various application fields the setup of a well-controlled synthesis route is needed. High vacuum conditions provide a well-defined reaction environment. A possible synthesis route to polymeric phthalocyanine sheets consists in the reaction of 1,2,4,5 tetracyanobenzene with a metal or metal salt. To achieve control over the reaction and, hence obtain optimized products, the understanding of the reactant behavior under high vacuum conditions is essential. Critical points that have to be considered are the sticking of the molecules on the substrate and the quartz microbalance during the PVD process, compound vapor pressure as well as side-reactions even during heating of the source.

CPP 50.36 Wed 18:30 P3

Absorption Tails of Donor:C_{60} Blends Provide Insight into Thermally Activated Charge-Transfer Processes and Polaron Relaxation — •Johannes Benduhn[1], Sebastian Schellhammer[2], Fortunato Piersimoni[3], Dieter Neher[3], Donato Spoltore[1], Frank Ortmann[2], and Koen Vandewal[1] — [1]IAP, TU Dresden — [2]Institute for Materials Science and cfaed, TU Dresden — [3]University of Potsdam

In organic semiconductors, the transfer of a localized charge carrier causes a deformation of the molecular structure, quantified by the intra-molecular relaxation energy. Such structural relaxation occurs upon forming intermolecular charge-transfer (CT) states at organic electron donor (D)-acceptor (A) interfaces. D-A complexes show weak absorption at photon-energies below the optical gap of both the donor and the C_{60} acceptor, which is the result of an optical transition from the neutral ground state to the ionic CT state. We show that temperature-activated intra-molecular vibrations of the ground state play a major role in determining the line-shape of such CT absorption bands, allowing to extract values for the relaxation energy. Those experimental values for 20 donor:C_{60} CT complexes correlate with values calculated within density functional theory. These results provide an experimental method for determining the polaron relaxation energy in solid-state organic D-A blends and show the importance of a reduced relaxation energy for thermally activated CT processes.

CPP 50.37 Wed 18:30 P3

Direct Observation of Intraband Relaxation and Exciton Dispersion Relation in Perylene-diimide H-aggregates — •Wouter Koopman[1], Stefano Toffanin[2], and Michele Muccini[2] — [1]Universität Potsdam, Potsdam, Deutschland — [2]CNR-ISMN, Bologna, Italien

The excited state properties of organic molecular solids are determined by the aggregation behavior of the constituent molecules. In extreme cases of J- and H-aggregates super-radiance or a complete suppression of photoluminescence can be observed. Here we report the direct observation of the intraband relaxation of H-aggregate excitons in a PTCDI-C13 thin film, by time resolved photoluminescence spectroscopy.

CPP 50.38 Wed 18:30 P3

Analysis of charge transfer states at organic single crystal interfaces — •Sebastian Hammer[1] and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

The formation, dissociation and recombination of charge transfer (CT) states at organic-organic interfaces are vital for the performance of organic opto-electronical devices. However, the energy and dynamics of CT-states strongly depend on the position of the participating molecular frontier orbitals as well as on their respective spatial arrangement.

Therefore, we have chosen chemically and structurally well-defined hetero-interfaces, comprised of organic single crystal surfaces and vacuum deposited molecular adsorbant layers, to analyze the efficiency of CT-state generation and the effective amount of transferred charge. For this purpose, various optical techniques such as locally resolved Raman spectroscopy are applied. In case of the latter, the amount of transferred charge is estimated by the linear frequency shift of selected molecular vibrational modes [1].

The methodical and analytical procedure is demonstrated for the model system Rubrene/C_{60} at different temperatures and crystallographic orientations.

[1] Matsuzaki, S. et al., *Solid State Commun.* **33**, 403 (1980)

CPP 51: Poster: Charged Soft Matter, Polyelectrolytes, Ionic Liquids

Time: Wednesday 18:30–21:00 Location: P3

CPP 51.1 Wed 18:30 P3

In situ small angle X-ray scattering investigation of solid-state polymer electrolyte for lithium-ion batteries — •Gilles Möhl[1], Ezzeldin Metwalli[1], Bernhard Springer[1], Rune Johnsen[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]TU Denmark, Department of Energy Conversion and Storage, Roskilde, DK-4000

Many present problems regarding the safety of liquid electrolytes in lithium-ion batteries may potentially be overcome by the use of solid-state polymer electrolytes. Polystyrene-block-polyethylene oxide PS-b-PEO diblock copolymer (DBC) electrolyte have been recently investigated as a membrane for Li-ion battery. The performance of these DBC electrolytes strongly depends on its morphology, serving highly oriented PEO domains as pathways for lithium ions migration. Thus, in situ structural investigation of these Li-ion doped DBCs systems during (dis)charge cycling in an operating battery is essential. A capillary-based micro-battery cell allowing simultaneous structural and electrical evaluation has previously been reported [1]. The current in situ small-angle X-ray scattering (SAXS) study of the solid-state polymer electrolytes using a modified version of the micro-battery cell provides a deeper insight into the possible structural modification and thus, on the involved conduction mechanisms during battery operation.

[1] R.E. Johnsen, P. Norby, J. Appl. Cryst. 2013, 46, 1537.

CPP 51.2 Wed 18:30 P3

In situ SANS investigation of block copolymer electrolyte under lithium stripping/platting cycling — •Bernhard Springer[1], Ezzeldin Metwalli[1], Robert Cubitt[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85478 Garching — [2]ILL, 6 rue Jules Horowitz, 38042 Grenoble, France

Due to safety concerns, solid-state electrolytes have recently garnered a great interest to replace liquid electrolytes. The conductivity and morphology of the solid-state lithium-salt containing polystyrene-block-polyethylene oxide (dPS-b-PEO) diblock copolymer (DBC) electrolyte are investigated during lithium metal stripping/platting cycling at different temperatures. The in situ small angle neutron scattering (SANS) measurements were performed on electrolytes, which are sandwiched between two thin lithium electrodes. Cylindrical morphology with interpenetrated nano-domains of both, the PS and PEO/Li-ion is observed. During cycling, the morphology of the system showed nearly no changes for temperatures up to 35°C, indicating good intrinsic stability. At higher temperatures $> 50°$C, a slight change in the inter-domain spacing indicates only a slight change in morphology. Interestingly, the level of domain alignment is significantly enhanced. The possible migration of the lithium ions during the galvanostatic cycling seems to open pathways between the two electrodes so that at high enough temperatures the domain re-orientation is favored. Our results imply that possible dendrite formation is highly suppressed for the employed solid-state electrolyte.

CPP 51.3 Wed 18:30 P3

Charge transport in monomeric vs. polymerized ionic liquids — •Felix Wieland[1], Wolf Hiller[2], Alexei Sokolov[3], Roland Böhmer[1], and Catalin Gainaru[1] — [1]Fakultät Physik, Technische Universität Dortmund, D-44221 Dortmund, Germany — [2]Fakultät für Chemie und Chemische Biologie, Technische Universität Dortmund, D-44221 Dortmund, Germany — [3]Department of Chemistry, University of Tennessee, Knoxville, Tennessee 37996, USA

Polymerized ionic liquids have been recently receiving the attention of scientific community as potential candidates for energy-storage materials in industrial applications [1] but also as testing ground for polymer research in general. In this work we analyze the variation of charge dynamics in monomeric, oligomeric, and long-chain ionic melts by means of dielectric spectroscopy, rheology, and field-gradient nuclear magnetic resonance. In this respect the length of the positively charged backbone is systematically increased while the type of anions and their concentration are kept invariant. Surprisingly, indications of a clear decoupling between the dynamics corresponding to positive and negative charges occur already for oligomeric chains comprising two to three monomeric units only. Our investigation aims at describing the evolution of transport parameters with the degree of polymerization and also at providing a general picture of the conductivity mechanism in ionic and polymerized ionic liquids [2].

[1] Fan, F. et al. Macromolecules 48 (13), 4461-4470 (2015). [2] Gainaru, C. et al. J. Phys. Chem. B 120 (42), 11074-11083 (2016).

CPP 51.4 Wed 18:30 P3

Effect of weakly/strongly interacting cation mixtures on LCST-LLPS in protein solutions — •Olga Matsarskaia[1], Nirzari Ann[1], Felix Roosen-Runge[2], Johannes Möller[3], Fajun Zhang[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]Institut Laue-Langevin, Grenoble, France — [3]ESRF, Grenoble, France

In the presence of trivalent cations, negatively charged globular proteins show a rich phase behaviour including reentrant condensation, crystallisation, clustering [1] and lower critical solution temperature metastable liquid-liquid phase separation (LCST-LLPS) [2]. Here, we present a systematic study of the influence of mixtures of varying ratios of Ho^{3+}/La^{3+}. Small-angle X-ray scattering (SAXS) data reveal that the interaction between BSA and the small cation Ho^{3+} is very strong, while the large La^{3+} interacts only weakly, which can be partly attributed to cation size effects. Using a combination of temperature-dependent UV-Vis as well as ζ potential measurements, we furthermore show that an increasing Ho^{3+}/La^{3+} ratio systematically shifts the LCST to lower values. Our findings imply that cation size and other cation-specific effects can be a sensitive tool to fine-tune protein-protein interactions and phase behaviour in solution.

[1] Zhang *et al.* Pure & Appl. Chem. 2014, 86, 191-202; [2] Matsarskaia *et al.* JPCB 2016, 120, 7731-7736.

CPP 51.5 Wed 18:30 P3

Solvent isotope effect on protein phase behavior in aqueous protein solutions — •Michal K. Braun[1], Marcell Wolf[1], Olga Matsarskaia[1], Stefano Da Vela[1], Felix Roosen-Runge[2], Michael Sztucki[3], Roland Roth[4], Fajun Zhang[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]ILL, Grenoble, France — [3]ESRF, Grenoble, France — [4]Institut für Theoretische Physik, Universität Tübingen

Knowledge about interactions and phase behavior of proteins in aqueous solutions is crucial in fields like protein crystallization, drug design and treatment of diseases. For many spectroscopic techniques in protein science D_2O is commonly used instead of H_2O in order to improve the signal. Here we present our finding of a strong solvent isotope effect on the protein phase behavior and the effective interactions in solutions of bovine serum albumin (BSA) with trivalent salts [1]. At intermediate salt concentrations the phase diagram exhibits a regime where condensation occurs [2]. This regime is significantly broadend when H_2O is replaced by D_2O. The lower critical solution temperature of liquid-liquid phase separation decreases significantly when D_2O is added to the solvent. Small angle x-ray scattering (SAXS) data shows that the reduced second virial coefficient is lower in D_2O than in H_2O. Both the macroscopic observations as well as the microscopic results consistently show that the attraction between the protein molecules increases when H_2O is replaced by D_2O.

[1] Braun et al., *in preparation*

[2] Zhang et al., *Pure Appl. Chem.*, **86**, 191, 2014

CPP 51.6 Wed 18:30 P3

Morphology of lithium-ion containing block copolymer electrolytes for rechargeable lithium-ion batteries — •Yinong Zhang, Ezzeldin Metwalli, Bernhard Springer, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Block copolymers (BC) electrolytes have been recently investigated as solid-state membranes for lithium-ion batteries. Nanostructured BC electrolyte contains both, the ionic conducting as well as the high-tensile polymer domains, enabling both, high ionic conductivity and improved mechanical stability. Since the diffusion path of the lithium-ions only follows the percolation path of the ionic conducting domain, the morphology of the BC electrolyte is an essential parameter. Theoretical studies have recently reported that the BC electrolyte phase diagrams significantly deviate from the conventional BC phase diagrams due to electrostatic interactions between polar chains and the alkali metal-ions. The morphology of ion-containing BC electrolyte was investigated using SEM and SAXS. In the current study, morphological deviation compared with that of the conventional BC phase diagrams in consistent with the theoretical studies is experimentally proved. Conductivity measurements of the Li-salt containing BC hybrid films were examined for different morphologies using impedance spectroscopy.

CPP 51.7 Wed 18:30 P3

Nanoporous titania/silica hybrid electrodes for lithium-ion batteries — •Kejie Zhang, Ezzeldin Metwalli, Thomas Kaps, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Light-weight, high energy density, stable and flexible solid-state lithium ion micro-batteries are of great importance due to its applications for miniature medical devices such as capsule endoscopes, implantable heart pumps and biosensors. The sol-gel template method synthesized nanostructured hybrid flexible thin film electrodes of titania (TiO2) with silica (SiO2) are expected to inherit titania's high charge/discharge rate, stability and good cyclability with silica's high gravimetric capacity and low potential. Different ratio of TiO2/SiO2 porous electrodes were prepared using different ratios of precursors and different weight ratio of polystyrene-block-polyethylene oxide (PS-b-PEO) diblock copolymer (DBC) guiding template. Here, lithium salt doped DBC is sandwiched between a developed TiO2/SiO2 anode and typical lithium cobalt dioxide cathode. Charge/discharge cycling capacity and impedance measurements after each cycle were acquired to characterize the stability, cyclability and capacity development of the assembled lithium-ion microbatteries. Small and wide angle X-ray scattering (SAXS/WAXS) were used for determination of the structures of free-standing TiO2/SiO2 nanoporous hybrid electrodes. The structure-property correlation of these hybrid electrodes are discussed.

CPP 51.8 Wed 18:30 P3

Specific Ion Effects on the Interfacial Structure and Foam Properties of Polystyrene Sulfonate Solutions — •Felix Schulze-Zachau and Björn Braunschweig — Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

Poly(sodium 4-styrenesulfonate) (NaPSS, 70 kDa) modified air/water interfaces were investigated with tensiometry, ellipsometry and vibrational SFG spectroscopy. Specific ion effects of K^+, Ca^{2+} and Nd^{3+} on the interfacial structure and adsorption properties of 20 mM NaPSS were studied. For a better understanding of the behavior in the bulk phase, turbidity measurements were performed. In order to relate the molecular structure of NaPSS in the bulk and at the interface to macroscopic foam properties, foams of these mixtures were analyzed with respect to their stability and structure. SFG spectra reveal charge screening with increasing ionic strength which is more effective for higher charged ions and linked with high foam stability. For Ca^{2+} ions, a change in the intensity ratio of CH_2/CH_3 vibrational bands can be related to a change in molecular structure at low salt concentrations. Structural changes in the foams can be linked to this change of molecular structure as we observe a bimodal bubble size distribution which is connected with poor foam stability. With increasing ionic strength, a decrease in surface tension and an increase of adsorbate thickness as well as foam stability is observed. The reason for that is charge screening and formation of aggregates which stabilize the foam bubbles and give rise to small mean bubble sizes.

CPP 51.9 Wed 18:30 P3

Scaling laws and solution rheology of semiflexible polyelectrolyte carboxymethyl cellulose: influence of electrostatic and hydrophobic interactions — •Carlos Lopez[1], Peter Graham[2], Ralph Colby[3], and Joao Cabral[1] — [1]Department of Chemical Engineering, Imperial College London, London SW7 2AZ, United Kingdom — [2]Unilever Research Port Sunlight Laboratory, Quarry Road East, Bebington L63 3JW, United Kingdom — [3]Department of Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania 16802

We investigate the conformation and rheology of sodium carboxymethyl cellulose (NaCMC) solutions. Scaling laws for the overlap and entanglement concentrations are established in salt free, NaCl and NaOH solutions. NaCl screens electrostatic interactions but not hydrophobic ones, while NaOH screens both. In salt free and NaCl solution, a highly substituted sample displays typical polyelectrolyte and neutral polymer in good solvent behaviour respectively. The viscosities in NaOH solutions are similar to those in NaCl. Less substituted samples display hydrophobic behaviour in salt free and NaCl solution, becoming thixotropic gels at high concentrations. However, the viscosities in NaOH are identical to those of the more substituted sample due to solubilisation of unsubstituted cellulose patches.

By varying the ionic strength and pH of aqueous solutions, it is possible to tune the polymer-solvent interactions for NaCMC samples. This allows us to separate the effects of entanglements, electrostatic and hydrophobic interactions on the solution rheology of NaCMC.

CPP 51.10 Wed 18:30 P3

Annealing in polyelectrolyte multilayers: influence of entanglements — Peter Nestler, Malte Passvogel, Annkatrin Sill, •Amir Azinfar, and Christiane A. Helm — Inst. of Physics, Greifswald University, Germany

Polyelectrolyte multilayer films were assembled by the layer-by-layer (LbL) technique using poly(stryrene sulfonate) PSS as polyanion and poly (diallyldimethylammonium) (PDADMA) as polycation. The first compartment of the film is built with protonated PSS, the second compartment with deuterated PSSd. The films were annealed in 1 M NaCl and the time dependent intermixing recorded with neutron reflectivity. If the layers are adsorbed from 0.1 M NaCl, the largest diffusion constant is found for M_w(PDADMA) = 45 kDa. If M_w(PDADMA) was lower, so was the diffusion constant. If M_w(PDADMA) was higher, then the diffusion constant dropped by two orders of magnitude. These findings suggest the diffusion of PDADMA/PSS complexes. The largest diffusion constant was obtained if the salt concentration of the preparation solution was decreased (0.03 M, 0.005 M). At low salt concentrations, less polyelectrolyte adsorbs with each deposition step, and fewer entanglements occur. These results suggest that polycation/polyanion complex formation and polymer entanglements influence the diffusion constant within polyelectrolyte multilayers.

CPP 52: Poster: Hydogels, Microgels, Responsive Polymers

Time: Wednesday 18:30–21:00 Location: P3

CPP 52.1 Wed 18:30 P3

H_2O - D_2O exchange kinetics in PNIPAM based block copolymer films followed with in-situ neutron reflectivity — •Lucas Kreuzer[1], Tobias Widmann[1], Nuri Hohn[1], Kun Wang[1], Jean-Francois Moulin[2], Viet Hildebrand[3], André Laschewsky[3], Christine Papadakis[1], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, Fachgebiet Physik weicher Materie/Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]HZG at MLZ, Lichtenbergstr. 1, 85748 Garching — [3]Universität Potsdam, Institut für Chemie, Karl-Liebknecht-Straße 24-25, 14476 Potsdam-Golm

Responsive polymers, especially in thin film morphology, are of great interest for a wide variety of applications where a strong change of volume is desired even for small changes of an external stimulus such as temperature. In this context the most prominent representative is poly(N isopropylacrylamide) (PNIPAM). We study a new block copolymer which comprises a PNIPAM block and a poly(sulfobetaine) (PSB) block. Thin films are prepared by spin coating on silicon substrates. We have followed the swelling of such films in water vapor atmosphere and found signature of H_2O - D_2O exchange in FT-IR data. We use neutron reflectivity to study the swelling behavior and the H_2O - D_2O exchange of PNIPAM-b-PSB films in more detail. In-situ neutron reflectometry enables to follow the kinetics and determine the underlying fundamental processes.

CPP 52.2 Wed 18:30 P3

In-Situ Neutron Reflectivity on H2O - D2O Exchange Kinet-

ics of Cross-Linked PNIPAM Microgel Thin Films — •Tobias Widmann[1], Lucas P. Kreuzer[1], Nuri Hohn[1], Kun Wang[1], Jean-François Moulin[2], Yvonne Hertle[3], Thomas Hellweg[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]HZG at MLZ, Lichtenbergstr. 1, 85748 Garching — [3]Bielefeld University, Physical and Biophysical Chemistry, Universitätsstr. 25, 33615 Bielefeld

Strong volume shifts of polymer thin films due to small modifications of an external stimulus like temperature are desired for a number of applications such as thermoresponsive nanoswitches or drug delivery in medicine. In this context the polymer which received most attention so far is poly(N-isopropylacrylamide), PNIPAM. The volume shift arises due to the collapse transition of the polymer at a lower critical solution temperature (LCST) which manifests in a swelling or deswelling of the polymer with water from its surroundings. To further our understanding of the kinetics of water uptake, release and exchange and the induced changes of the polymer properties, microgel thin films from a PNIPAM homopolymer with varying amounts of N,N'-Methylenebisacrylamide cross-linkers are prepared. In-situ neutron reflectometry in time of flight (TOF) mode is used to investigate the uptake and exchange kinetics of H2O with D2O and vice-versa for these films at temperatures below the LCST of PNIPAM.

CPP 52.3 Wed 18:30 P3

Polymer microgels in cell-free biotechnology — •Max Männel, Nicolas Hauck, Thomas Heida, Ivan Raguzin, Anika Kaufmann, Andreas Fery, and Julian Thiele — Leibniz-Institut für Polymerforschung Dresden e. V., Leibniz Research Cluster, Germany

The formation of microemulsions in microfluidic flow cells, termed droplet microfluidics, has been established as highly modular method for the fabrication of polymer microgels. The microfluidic flow cells are commonly fabricated by a combination of photo- and soft lithography using poly(dimethylsiloxane) (PDMS). A promising alternative which is less expensive and time-consuming is additive manufacturing, also referred to as 3D printing, which allows the fabrication of flow cells in an affordable, high-resolution and fast single-step process. Our investigated polymer microgels are formed by crosslinking thiol-functionalized hyaluronic acid (HASH) and poly(ethylene glycol) diacrylate (PEGDA) via mild thiol-Michael addition. These microgels have various applications in cell-free biotechnology since they provide a controllable reaction environment. One topic of intense research in our group is the immobilization of enzymes for the production of novel, non-natural pharmaceuticals, e. g. polyketides. Another relevant process in biotechnology is the cell-free protein synthesis which can be realized by attaching DNA to the same polymer microgels. Performing these reactions in microfluidic bioreactors with various reaction chambers and a continuous flow allow the production of seldom products which can not be fabricated by conventional processes.

CPP 52.4 Wed 18:30 P3

Optimization of Planar Hydrogel-Based Micro-Valves for On-Chip Flow Control — •Anthony Beck, Philipp J. Mehner, Georgi Paschew, Martin Elstner, and Andreas Richter — Chair of Polymeric Microsystems, Technische Universität Dresden, Germany

A successful miniaturization and commercialization of fully integrated microfluidic systems are still under development due to the lack of reliable microfluidic components like micro-valves. Feasible hydrogel-based micro-valve concepts have been demonstrated and show a promising potential for high integration lab-on-chip applications. Due to the vast amounts of synthesis and design parameters an experimental development of reproducible, low-response micro-valves have only been done insufficiently. We propose a systematic investigation of a temperature triggered, hydrogel-based, planar micro-valve. Experimentally, the channel shapes, number and geometry of hydrogel elements have been evaluated to improve performance parameters. Furthermore, different MEMS compatible manufacturing techniques are assessed. Additional modifications allow the development of one-directional valves with a diode-like behavior. Computer aided models describes physical design parameters which are implemented in the current concepts. The proposed design changes improve the valve response time and break through pressures of up to 1 bar and formulate new design rules for next generation micro-valves.

CPP 52.5 Wed 18:30 P3

In-situ soft X-ray analysis of various polymer-based microcontainers for theranostic and catalytic applications — •Andreas Späth[1], Gaio Paradossi[2], George Tzvetkov[3], and Rainer H. Fink[1] — [1]Friedrich-Alexander Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II and ICMM, Erlangen, Germany — [2]Universita di Roma Tor Vergata, Dipartimento di Scienze e Tecnologie Chimiche, Rome, Italy — [3]University of Sofia, Department of Inorganic Chemistry, Sofia, Bulgaria

Polymer-based microshells and microgel particles are versatile containers for the transport of drugs, theranostic gases or catalytically active molecules. They are in many cases biodegradable and fully compatible to in-vivo applications. During recent years we have investigated a broad range of such hybrid materials ranging from gas filled microballoons and thermoresponsible microgel networks to magnetoresponsive particles with embedded iron nanoparticles and core-shell systems with various fillings, e.g., ionic liquids [1-3]. Soft X-ray microscopy is an excellent tool to study those systems in-situ in aqueous matrix with high-resolution and chemical sensitivity. We have analyzed shell thicknesses, swelling behaviors and responses to temperature increase to contribute better understanding on release mechanisms, have developed procedures to derive 3D representations of the particles from originally 2D transmission micrographs.

[1] A. Späth et al., Ultramicroscopy, 2014, 144, 19.
[2] A. Späth et al., RSC Advances, 2014, 4, 3272.
[3] A. Späth et al., RSC Advances, 2016, 6, 98228.

CPP 52.6 Wed 18:30 P3

Aggregation behavior of PNIPAM in dependence on temperature and pressure — •Bart-Jan Niebuur[1], Kora-Lee Claude[1], Simon Pinzek[1], Konstantinos N. Raftopoulos[1], Vitaliy Pipich[2], Marie-Sousai Appavou[2], Alfons Schulte[3], and Christine M. Papadakis[1] — [1]Technische Universität München, Physik-Department, Fachgebiet Physik weicher Materie, Garching, Germany — [2]Jülich Centre for Neutron Science JCNS, Forschungszentrum Jülich GmbH, Outstation at MLZ, Garching, Germany — [3]University of Central Florida, Department of Physics and College of Optics & Photonics, Orlando, U.S.A.

The phase separation mechanism of poly(N-isopropylacrylamide) (PNIPAM) is still under debate. Instead of phase separating macroscopically, PNIPAM forms stable mesoglobules in the two-phase region at atmospheric pressure in aqueous solutions. We have investigated the phase behavior in dependence on temperature and pressure using turbidimetry. The aggregates in the two-phase region are characterized using very small-angle neutron scattering, optical microscopy and Raman spectroscopy. At high pressure, the aggregates are larger than at atmospheric pressure. A possible reason is the decreased efficiency of the phase separation at high pressure because the chains stay hydrated even in the two-phase region. Thus, inducing the phase transition by applying high pressure and by combining a variety of methods, the nature of the transition can be related to the mesoscopic domain structure in the two-phase state.

CPP 52.7 Wed 18:30 P3

Poly(NIPAm) can actuate to stable 3D forms: An experimental-numerical study on one component dual actuation — •Ali Ghaemi[1], Li Liu[2], Stephan Gekle[1], and Seema Agarwal[2] — [1]Biofluid Simulation and Modeling, Fachbereich Physik, and Bayreuth Center for Colloids and Interfaces, Universität Bayreuth, Universitätsstraße 30, 95440 Bayreuth, Germany — [2]Macromolecular Chemistry II and Bayreuth Center for Colloids and Interfaces, Universität Bayreuth, Universitätsstraße 30, 95440 Bayreuth, Germany

Numerical analysis in combination with experimental results are applied in order to explain the complex behavior of a rare example of one-component dual actuators. The system of interest is a bilayer with aligned and randomly oriented poly(N-isopropyl acrylamide) fibers which displays irreversible change in shape by rolling in contact with water, and reversible size change in response to temperature changes. A combination of anisotropic Young*s modulus and temperature dependent swelling/shrinkage was shown to be responsible for the actuators controllable unique folding.

CPP 52.8 Wed 18:30 P3

Phase transition and aggregation behaviour of an UCST-type copolymer Poly(Acrylamide-co-Acrylonitrile) in Aqueous Media — Asad Asadujjaman[1], Ben Kent[2], and •Annabelle Bertin[1,3] — [1]Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany — [2]Helmholtz-Zentrum Berlin (HZB), Hahn-Meitner-Platz 1, 14109 Berlin, Germany —

[3]Freie Universität Berlin, Institut für Chemie und Biochemie, Takustr. 3, 14195 Berlin, Germany

Thermoresponsive polymers have shown great potential in applications such as bioseparation, drug delivery and diagnostic.[1-2] Only few thermoresponsive polymers that present an upper critical solution temperature (UCST), i.e. phase separate from solution upon cooling, in a relevant temperature range have been reported so far. Herein, a robust UCST-type copolymer of acrylamide (AAm) and acrylonitrile (AN) (poly(AAm-co-AN)) was prepared by reversible addition fragmentation chain transfer (RAFT) polymerization and its thermo-induced aggregation behavior in aqueous media was studied.[1,2] We propose a model for the temperature-induced aggregation behaviour of UCST-type poly(AAm-co-AN) copolymer in aqueous solution on the basis of turbidity measurements, SLS, DLS, SANS and cryo-TEM. [1] Asadujjaman A., Kent B., Bertin A., Soft Matter, 2016, accepted. [2] Asadujjaman A., Bertin A., Schönhals A., Soft Matter, 2016, submitted.

CPP 52.9 Wed 18:30 P3

Functional polymers based on diaminopyridine motif with tunable UCST behavior in alcohol and water/alcohol mixtures — Asad Asadujjaman[1], Vahid Ahmadi Soureshjani[1], Meral Yalcin[2], Niels ten Brummelhuis[2], and •Annabelle Bertin[1,3] — [1]Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany — [2]Humboldt Universität zu Berlin, Department of Chemistry, Brook-Taylor-Str. 2, 12489 Berlin, Germany — [3]Freie Universität Berlin, Institute of Chemistry and Biochemistry, Takustr. 3, 14195 Berlin, Germany

Thermoresponsive polymers are of great importance in numerous applications such as bioseparation, drug delivery, diagnostic and microfluidic applications. Only few thermoresponsive polymers that present an upper critical solution temperature (UCST), i.e. phase separate from solution upon cooling, in a relevant temperature range and green solvents such as water or ethanol have been reported. Indeed, polymers with UCST behavior below 60°C in alcohol or water/alcohol mixtures are extremely promising for the preparation of smart materials for sensing. In this work two novel functional polymers of based on a 2,6-diaminopyridine motif were synthesized by free radical polymerization. Their UCST-type transition temperature is tunable by varying either their concentration in solution or the type of solvent. Insights into this phenomenon will be given based on turbidimetry and temperature dependent dynamic light scattering.

CPP 52.10 Wed 18:30 P3

Smart Binary Polymer Brush Surfaces For Controlled Biocatalysis — •Alice Rosenthal[1,2], Sebastian Rauch[1], Klaus-Jochen Eichhorn[1], Manfred Stamm[1], and Petra Uhlmann[1,3] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., PF 120411, 01005 Dresden — [2]Technische Universität Dresden, 01062 Dresden — [3]Department of Chemistry, Hamilton Hall, University of Nebraska-Lincoln, 639 North 12th Street, Lincoln, Nebraska 68588, United States

Polymer brushes represent smart surfaces due to their ability to respond to changes in the environmental conditions (e. g. temperature) by showing a reversible swelling-deswelling behavior. Moreover, polymers with functional groups offer a way to immobilize enzymes in an active manner. By combining polymers with opposite properties, switching between different states depending on the external conditions becomes feasible. We fabricated binary polymer brushes consisting of the Poly(N-isopropylacrylamide) (PNIPAAm) and Poly(ethylene glycol) (PEG). In contrast to PEG, PNIPAAm exhibits a lower critical solution temperature (LCST) close to the physiological range (31 °C). In-situ spectroscopic ellipsometry was used to investigate the temperature-responsive swelling behavior of the binary brushes in comparison to the respective homo-brushes. Horseradish Peroxidase conjugated Streptavidin (SA-HRP) was immobilized through accessible alkyne groups at the outer extremity of the PNIPAAm chains. For the enzyme modified binary PNIPAAm/PEG brushes, the enzymatic activity can be switched between an active state at 20°C and a less active state at 40°C in aqueous medium.

CPP 52.11 Wed 18:30 P3

Mixed polymer brushes with complex pH- and temperature-sensitivity and tunable protein adsorption capability — •Stefan Adam[1,2], Klaus-Jochen Eichhorn[1], Frank Simon[1], Manfred Stamm[1,2], and Petra Uhlmann[1,3] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany. — [2]Technische Universität Dresden, 01062 Dresden, Germany. — [3]University of Nebraska-Lincoln, Lincoln, NE 68588, USA.

Responsive polymer coatings or hydrogels can change their structural and physical properties due to external stimuli (e.g. temperature or pH). When combining polymers responding to different triggers, systems with new properties such as dual- up to multi-responsiveness can be created. We investigated the complex pH- and temperature-sensitive swelling behavior of mixed polymer brushes comprising pH-responsive poly(acrylic acid) (PAA) and a thermo-responsive poly(2-oxazoline) (POX) in water using in situ spectroscopic ellipsometry. Mixed brushes of varying compositions were prepared via a *grafting to* approach by sequential anchoring of both polymers. All binary brushes exhibit an amplified pH-sensitivity compared to PAA brushes as well as a temperature-sensitivity at sufficient high POX content and at pH>4. Angle-resolved X-ray photoelectron spectroscopy measurements were performed to get deeper insights into changes in the vertical brush composition caused by differences in the external environment, the brush composition and the preparation sequence. Such dual-responsive mixed brushes are promising for tuning the protein adsorption, as it could be proven for bovine serum albumin as a model protein.

CPP 52.12 Wed 18:30 P3

Electroactive silicone gel layers with tailor made actuation behavior for tunable mirrors — •Markus Franke[1], Irma Slowik[2], Philipp Mehner[1], Ulrich Merkel[1], Hartmut Fröb[2], Karl Leo[2], and Andreas Richter[1] — [1]Institut für Halbleiter- und Mikrosystemtechnik, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Dresden Integrated Center for Applied Physics and Photonic Materials, Technische Universität Dresden, George-Bähr-Strasse 1, D-01069 Dresden, Germany

The research field of electroactive polymers (EAP) enables varied applications in robotics, energy harvesting, sensing or even tunable optics. Here, a utilization of EAP actuators for tuning optical mirrors can be a cost- and process-efficient alternative to current membrane based MEMS. In this study we developed various silicone gel based EAP actuators for tuning highly reflecting mirrors. They consist of a thin and structured silver layer acting as a flexible top electrode, a compressible silicone layer and a fixed ground electrode. This capacitor setup allows a tailor made EAP actuation and mirror deflection in height or angle by varying processing parameters like crosslinking density of the gel, surface activation or lateral dimension of the electrode. These aspects could be clarified by surface analysis as well as electrical and mechanical characterization of the EAP actuator. Furthermore, finite element simulation helps to understand the versatile mirror deflection shapes depending on the mechanical strength or the electrical field distribution of the capacitor. Finally, the EAP actuator with a planar shaped mirror deflection is applied for a tunable optical micro cavity setup.

CPP 53: Keynote Lecture III

Time: Thursday 9:30–10:00 Location: ZEU 222

Invited Talk CPP 53.1 Thu 9:30 ZEU 222
Interplay of Order and Disorder in Self-assembled Optical Metamaterials — •Ullrich Steiner — Adolphe Merkle Institute

Metamamaterials are periodic structural arrays that allow the propagation of radiation in a fashion that is not observed in other systems, most notably a negative refractive index and super-focussing properties. The creation of metamaterials for visible light involves the manufacture of 3D arrays from plasmonic metals (gold, silver) with sub-100 nm periodicities. While micrometer-sized metamaterials for microwave and infrared-radiation can be lithographically manufactured, novel approaches are required for metamaterials that operate as visible wavelength.

In my presentation, I will introduce a concept that makes use of polymer self-assembly. Structurally chiral materials that form by self-assembly are replicated into gold and their optical properties are investigated. This leads to the creation of periodic plasmonic materials with an exceptional transparency for for optical wavelengths and interesting circular and linear dichroism.

Since the optical properties of these nanostructured materials depend sensitively on the structural symmetry of the self-assembled lattice, special attention will be paid to the control of gyroid self-assembly in thin films, and how the perfection (or lack-therof) of the self-assembled morphology affects the optical properties of the material.

CPP 54: Active Matter II (joint session DY/BP/CPP, organized by DY)

Time: Thursday 9:30–13:00 Location: HÜL 186

Invited Talk CPP 54.1 Thu 9:30 HÜL 186
Rolling, rolling, rolling – a new self-propulsion mechanism — •Falko Ziebert[1,2] and Igor Kulic[2] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, 79104 Freiburg, Germany — [2]Institut Charles Sadron UPR22-CNRS, 67034 Strasbourg Cedex 2, France

We describe a generic mechanism that induces an instability towards rolling motion of a rod along a heated plate. The mechanism, relying on geometric planar confinement, can be explained by an effective model combining elasticity of a rod with thermal advection-diffusion. We exemplify the versatility of the effect by investigating self-propellers, as well as simple motors and energy storage devices, both experimentally and theoretically.

CPP 54.2 Thu 10:00 HÜL 186
Cluster Formation and Deformation of Spherical Circle Swimmers Dispersed on a Monolayer — •Guo-Jun Liao and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin

Inspired by recent experimental developments in manufacturing "active" colloidal particles with unusual, e.g. curved, modes of motion (such as form-anisotropic particles [1] or decorated metallodielectric Janus spheres [2]), as well as by the proceeding of a theoretical study on the collective behavior of curved polymers with circular paths [3], we computationally investigate models of spherical particles in which the colloids dispersed on a monolayer feel not only a propelling force, but also a propelling torque. In the absence of propulsion torque (without circular motion), we find clustering of "conventional" self-propelled disks, in accordance with Ref. [4]. We show that the motility-induced cluster formation is enhanced by polar interaction, and cumulatively hindered by increasing the propulsion angular velocity ω_0. Different from the model of curved polymers [3], in which the occurrence of stable vortices is attributed to the shape anisotropy, our generic model of isotropic "active" spheres also form clockwise vortices as ω_0 approaches the rotational diffusion coefficient D_r.

[1] F. Kümmel et al., Phys. Rev. Lett. **110**, 198302 (2013)
[2] S. Gangwal et al., Phys. Rev. Lett. **100**, 058302 (2008)
[3] J. Denk et al., Phys. Rev. Lett. **116**, 178301 (2016)
[4] J. Bialke et al., EPL **103**, 30008 (2013)

CPP 54.3 Thu 10:15 HÜL 186
Effect of the orientational relaxation on the collective motion of patterns formed by self-propelled particles. — •Alexander Chervanyov[1], Hector Gomez[2], and Uwe Thiele[1] — [1]Institut für Theoretische Physik, WWU Münster, Germany — [2]Universidade da Coruna, A Coruna, Spain

We investigate the collective behavior of self-propelled particles (SPPs) undergoing competitive processes of pattern formation and rotational relaxation of their self-propulsion velocities. As a main result of this study, we quantitatively explain [1] transitions between different steady states of the SPPs caused by the intricate interplay among the involved effects of pattern formation, orientational order, and coupling between the SPP density and orientation fields. Based on rigorous analytical and numerical calculations, we prove that the rate of the orientational relaxation of the SPP velocity field is the main factor determining the steady states of the SPP system. Further, we determine the exact boundaries between domains in the parameter plane that delineate qualitatively different resting and moving states. In addition, we analytically calculate the collective velocity of the SPPs and show that it perfectly agrees with our numerical results. Our results can be effectively used to identify the regimes of collective behavior of SPPs in living systems in relevance to the domains of dominance of the above described effects of the self-propulsion, pattern formation and orientational relaxation of SPPs.

[1] A.I. Chervanyov, H. Gomez, U. Thiele, EPL 115, 68001 (2016).

CPP 54.4 Thu 10:30 HÜL 186
Statistical features of active turbulence — •Martin James and Michael Wilczek — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Dense bacterial suspensions display rich dynamical features including turbulence-like behavior. Recent studies have shown that such turbulent dynamics of active fluids can be modeled by a generalized Navier-Stokes equation (Wensink et al., PNAS 2012). The statistical features of active turbulence, however, differ significantly from classical hydrodynamic turbulence (see, e.g., Bratanov et al., PNAS 2015). We further explore the statistical features of this active turbulence model both, numerically and analytically. In particular, we focus on scale-dependent statistics to characterize deviations from Gaussianity and the occurrence of extreme events. Moreover, we investigate the transport properties of active flow by using Lagrangian tracer techniques. Our results provide insight into mixing of microbial suspensions due to turbulent dynamics.

CPP 54.5 Thu 10:45 HÜL 186
Large scale vortex-patterns in dense suspensions of microswimmers — •Sebastian Heidenreich[1], Jörn Dunkel[2], Sabine H. L. Klapp[3], and Markus Bär[1] — [1]Physikalisch-Technische Bundesanstalt — [2]Massachusetts Institute of Technology — [3]Technische Universität Berlin

In this talk we consider a prominent examples of an active biological fluid - dense suspension of swimming bacteria (e. g. Bacillus subtilis). For dense suspensions of bacterial swimmers, we have proposed a simple phenomenological model that predicts regular and turbulent vortex lattices and reproduces recent experimental findings of mesoscale turbulence in two- and three-dimensional suspensions of Bacillus subtilis in a quantitative manner [1]. A continuum model that couples the orientation of the swimmers with the surrounding velocity field was derived from stochastic equations of motions for individual active swimmers for a realistic hydrodynamical model of swimmers in a fluid [2]. This model contains the simple phenomenological model used in [1] as a special case. Furthermore, the continuum model enables us to understand the mechanism and properties of pattern formation in microswimmer suspensions and relate the physical parameters characterizing the individual swimmers and their interaction to the coefficients for continuum model equations.

[1] Dunkel, S. Heidenreich, K. Drescher, H. H. Wensink, M. Bär & R. E. Goldstein Phys. Rev. Lett. 110; New. J. Phys. (2013).

[2] S. Heidenreich, J. Dunkel, S. L. Klapp, and M. Bär (2016). Phys. Rev. E, 93

CPP 54.6 Thu 11:00 HÜL 186

Collective Effects of Active Particles at Fluid-Fluid Interfaces. — •Irina Kistner, Paolo Malgaretti, Mihail Nicolae Popescu, and Siegfried Dietrich — Max-Planck-Institut fuer Intelligente Systeme, Stuttgart, Germany

Micrometer sized particles capable of self-induced motility are of high interest for various applications in medicine, sensing and environmental science. Recent works report of different types of collective motion such as clustering, swarming or fluid-solid phase separation. Moreover different phenomena may arise when active particles are bounded or reside in the proximity of a fluid-fluid interface [1], [2].

The model system we are investigating consists of two or more chemically active, spherical colloidal particles located close to a fluid-fluid interface. Due to the Marangoni stresses self-induced at the interface, the particles experience a repulsive long-ranged effective force field under harmonic confinement. We show that this effective interaction results in a crystal-like pattern formation of collectively rotating particles and define a gas-crystal phase separation governed by the Marangoni force constant.

[1] A. Dominguez, P. Malgaretti, M. N. Popescu, and S. Dietrich: Effective interaction between active colloids and fluid interfaces induced by Marangoni flows, Phys. Rev. Lett. 117, 079902 (2016)

[2] A. Dominguez, P. Malgaretti, M. N. Popescu, and S. Dietrich: Collective dynamics of chemically active particles trapped at a fluid interface, Soft Matter, 12, 8398-8406 (2016)

15 min. break

CPP 54.7 Thu 11:30 HÜL 186

Mechanical Instabilities in Active Systems — •Christoph A. Weber and Lakshminarayanan Mahadevan — Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA

Active stress can affect the stability of biological systems and drive macroscopic changes of matter on very short time scales that cannot be explained by the liquid-like transport of the constituents. Examples are contracting active gels or the compaction of cells in tissues. For these systems the solid-like response to active stress is the key to understand the physics underlying the change of matter. Here we study a generic framework to describe mixtures composed of an active solid and a passive liquid phase. We find that such a mixture is unstable for large enough activity and can demix into regions mostly consisting of solid or fluid, respectively. The instability leads to the formation of disintegrated patches of a length scales which arises from the competition between the shear transport in the solid phase versus the solid-liquid momentum transfer. This mechanical instability might be relevant for many very dense active systems where liquid-like particle transport is mostly jammed.

CPP 54.8 Thu 11:45 HÜL 186

Defect dynamics in topological active matter — •Axel Voigt and Francesco Alaimo — Institute für Wissenschaftliches rechnen, TU Dresden

If active systems are confined on curved surfaces, topological constraints strongly influence the emerging spatiotemporal patterns. Using these topological constraints to guide collective cell behavior might be a key in morphogenesis and active nematic films on surfaces have been proposed as a promising road to engineer synthetic materials that mimic living organisms. Recent experiments consider an active nematic film of microtubules and molecular motors encapsulated within a lipid vesicle. As in passive systems the mathematical Poincare-Hopf theorem forces topological defects to be present in the nematic film. On a spherical vesicles this leads to an equilibrium defect configuration with four $+1/2$ disclinations arranged as a tetrahedron. In active systems unbalanced stresses drive this configuration out of equilibrium. But in contrast to planar active nematics with continuous creation and annihilation of defects the creation of additional defect pairs can be suppresses on curved surfaces. This led to the discovery of a tunable periodic state that oscillates between the tetrahedral and a planar defect configuration. We confirm this finding by computer simulations. For non-constant Gaussian curvature constraints local geometric properties can be used to control defect dynamics. We are concerned with a systematic investigation of the impact of such constraints on the emergence of complex patterns and oscillations.

CPP 54.9 Thu 12:00 HÜL 186

Dancing disclinations in living fluids — •Amin Doostmohammadi, Tyler Shendruk, Kristian Thijssen, and Julia Yeomans — University of Oxford

The spontaneous emergence of collective flows is a generic property of active fluids and often leads to chaotic flow patterns characterised by swirls, jets, and topological disclinations in their orientation field. However, the ability to achieve structured flows and ordered disclinations is of particular importance in the design and control of active systems. By confining an active nematic fluid within a channel, we find a regular motion of disclinations, in conjunction with a well defined and dynamic vortex lattice. As pairs of moving disclinations travel through the channel, they continually exchange partners producing a dynamic ordered state, reminiscent of Ceilidh dancing. We anticipate that this biomimetic ability to self-assemble organised topological disclinations and dynamically structured flow fields in engineered geometries will pave the road towards establishing new active topological microfluidic devices.

CPP 54.10 Thu 12:15 HÜL 186

Effective interactions between catalytic particle and fluid-fluid interfaces — •Paolo Malgaretti, Mihail Nicolae Popescu, and Siegfried Dietrich — Max Planck Institute for Intelligent Systems, Heisenbergstr. 3 70569 Stuttgart Germany

When catalytic particles, such as Janus particles, or enzymes are in the vicinity of a fluid-fluid interface, their is strongly modulated by the pres-ence of the interface and/or by the inhomogeneity in the transport properties of the two fluid phases. Hence, the effective interaction with the interface can lead to novel dynamical regimes absent in homogeneous fluids. For example, if the by-products of the catalysis are surfactants their spatial distribution will affect the local value of the surface tension. In such a scenario, when catalytic particles approache a fluid-fluid interface a Marangoni flow will set up in response to the inhomogeneity in the surface tension induced by the byproducts of the catalysis. The onset of such a flow attracts the catalytic particle towards the interface. Interestingly the strength of such an effective attraction is strongly affected by the affinity of the byproduct to the interface as well as by the transport properties of the two fluid phases. In particular, for water-oil interfaces such an effect overwhelms other means of active transport such as self-diffusiophoresis and makes it suitable to enhance particle accumulation close to fluid-fluid interfaces. Finally I will discuss the onset of collective behavior.

CPP 54.11 Thu 12:30 HÜL 186

Active crystals on the sphere — •Simon Praetorius[1], Axel Voigt[1], Raphael Wittkowski[2], and Hartmut Löwen[3] — [1]Institute of Scientific Computing, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Institut für Theoretische Physik Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany — [3]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf, Germany

Two-dimensional crystals on curved manifolds like a sphere exhibit nontrivial defect structures. Here we consider "active" crystals on the sphere which are composed of self-propelled particles. A coarse-grained model is proposed by unifying the Phase-Field Crystal approach with a Toner-Tu-like theory which involves a density and a polarization field on the sphere. Depending on the strength of the self-propulsion, four different dynamical modes are found: a resting crystal, a self-spinning "vortex-vortex" crystal containing two vortical poles with integer defects of the polarization, a "source-sink" crystal and a travelling/spinning lamellar. We analyze the dependence of orientational and translational defects on the activity of the crystal.

CPP 54.12 Thu 12:45 HÜL 186

Green-Kubo approach to active Brownian systems — •abhinav sharma and joseph Brader — Universite de Fribourg, Rue du Musee 3, ch 1700, Fribourg

We develop an exact Green-Kubo formula relating nonequilibrium averages in systems of interacting active Brownian particles to equilibrium time-correlation functions. The method is applied to calculate the density-dependent average swim speed, which is a key quantity entering coarse grained theories of active matter. The average swim speed is determined by integrating the equilibrium autocorrelation function of the interaction force acting on a tagged particle. We generalize our approach to a spatially and time varying activity. Analytical results are validated using Brownian dynamics simulations.

CPP 55: Focus: Static and Dynamic Disorder Phenomena on the Transport in Organic Semiconductors I

Organisers: Jens Pflaum (Universität Würzburg), Thomas Kirchartz (FZ Jülich), Dieter Neher (Universität Potsdam)

Transport of charge carriers as well as of excitons defines a crucial process in the successful implementation of organic semiconductors in modern thin-film applications. In particular, structural and energetic disorder influences the localization of charge carriers and excitons and, thus, exerts a tremendous influence on the nature of transport in small molecule as well as polymer semiconductors. However, as demonstrated by recent theoretical work, the correlation between disorder and charge transport becomes much more complex taking into account dynamic effects and their related time-scales. In certain cases, this might even lead to delocalization of previously localized charge carries, thereby being beneficial for the overall macroscopic transport. Therefore, this focus session aims for bringing together experimentalists as well as theoreticians working in the field of charge and exciton transport in organic materials. Only by complementary contributions from different areas in organic solid states, including rational design of materials, development of advanced methods and state-of-the-art calculations, a comprehensive understanding of the relationship between disorder and transport will be feasible and, thus, a successful application of advanced optimization strategies to real devices. As such, this focus session is intended to provide the suited platform for an intense informational exchange on this topic and, thereby, to initiate possible future collaborations between the relevant groups.

Time: Thursday 10:15–13:00 Location: ZEU 222

Invited Talk CPP 55.1 Thu 10:15 ZEU 222

Understanding charge transport in crystalline organic semiconductors — •Simone Fratini[1], Sergio Ciuchi[2], Alessandro Troisi[3], and Didier Mayou[1] — [1]Institut Néel - CNRS and Université Grenoble Alpes, Grenoble, France — [2]Department of Physical and Chemical Sciences, University of L'Aquila & CNR-ISC, L'Aquila, Italy — [3]Department of Chemistry, University of Warwick, UK

Charge transport in crystalline organic semiconductors is intrinsically limited by the presence of large thermal molecular motions, which are a direct consequence of the weak van der Waals intermolecular interactions. These lead to an original regime of transport called transient localization, involving the quantum localization of the carriers at timescales shorter than the typical molecular motions. After a brief review of experimental observations that pose a challenge to textbook theories, I will present model calculations supporting the transient localization scenario. I will show that the theory consistently explains several common experimental features of organic semiconductors, such as the low mobilities falling below the Mott-Ioffe-Regel limit, the typical power-law temperature dependence observed in clean crystalline compounds as well as the observed non-Drude like behavior of the optical conductivity. I will then discuss efficient strategies to improve the mobility in this important class of materials and conclude with a systematic screening performed on the whole family of organic semiconductors, showing how the electronic structure determines their sensitivity to molecular disorder. Mobilities above 100 cm^2/Vs are predicted to occur in appropriately tailored compounds.

Invited Talk CPP 55.2 Thu 10:45 ZEU 222

Mapping of trap densities and contact resistance in organic devices and their relation to structural disorder — •Bert Nickel[1], Clemens Liewald[1], Simone Strohmair[1], Eric Glowacki[2], and Andrey Turchanin[3] — [1]Ludwig-Maximilians-Universität, Department of physics & CeNS, D-80539 Munich, Germany — [2]Linköpings Universitet, Laboratory of Organic Electronics, SE-601 74 Norrköping, Sweden — [3]Friedrich-Schiller-Universität Jena, Institute of Physical Chemistry, 07743 Jena, Germany

We develop experimental tools to explore the influence of static and dynamical disorder phenomena on transport in organic devices. Examples studied range from simple aromatics such as pentacene and DNTT to H-bonded pigments such as epindolidione. We aim on correlating the electronic transport properties [1] with local structural properties obtained from nano beam x-ray diffraction experiments and near field microscopy [2]. Photocurrent microscopy allows us to determine local transport properties such as trap densities and charge carrier dynamics in fully operational thin film transistors, as well as local distribution of contact resistances. Contact resistance is often related to imperfect growth on metal contacts, we will present new approaches to deposit highly ordered films by transfer techniques.

[1] C. Liewald, D. Reiser, B. Nickel, Applied Physics Letters 109, p53301 (2016)

[2] C. Westermeier, A. Cernescu, S. Amarie, C. Liewald, F. Keilmann, B. Nickel, Nature Communications 5, Article Number 4101 (2014)

15 min break

CPP 55.3 Thu 11:30 ZEU 222

Construction of Polycrystalline Morphologies: A Case Study for C60 and Pentacene — •Sebastian Schellhammer[1,2,3], Frank Ortmann[1,2], and Gianaurelio Cuniberti[1,2,3] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden — [2]Dresden Center for Computational Materials Science, TU Dresden — [3]Center for Advancing Electronics Dresden, TU Dresden

Based on the processing conditions, the morphology of small-molecule organic semiconducting materials can be varied from highly ordered single crystals to polycrystalline and amorphous. Also grain shapes vary from spherical, platelets, or rod-like. Differences in the morphology affect the energy landscape and, thus, the macroscopic charge transport behavior of the film. We present a nucleation-equilibration approach for the construction of morphologies with gradually varying degree of structural ordering. Based on geometrical considerations, the computational requirements are low enabling the construction of systems of experimentally relevant sizes. Application is demonstrated for C60 and pentacene structures varying from almost amorphous to highly ordered phases. We will also discuss the impact of morphologies on charge transport.

CPP 55.4 Thu 11:45 ZEU 222

Dithienylethene as Switchable Hole Trap in Organic Semiconductors — •Tim Schaefer, Dirk Hertel, and Klaus Meerholz — Department of Chemistry, University of Cologne, Germany

Trap states can considerably hinder charge carrier transport. To better understand the influence of traps on the charge transport properties of organic semiconductors, we mix in traps on purpose. We present a unique hole trap, dithienlyethene (DTE), which can be photochemically switched "off" [1] to tune the trap concentration in one and the same device. DTE features two stable isomers that differ in HOMO energy. In a hole-conducting matrix with a certain HOMO energy, one DTE isomer acts as a hole trap, while the other isomer has a negligible influence on charge transport. The energetic trap depth is varied by blending DTE with various TPD-type hole conductors featuring different HOMO levels. In first proof-of-principle experiments, the hole mobility of the space-charge-limited current in a blend with DTE is reversibly switched by a factor of ca. 20. In contrast, in blends where DTE is replaced by a permanent trap with a similar trap depth trap-limited current is observed. Temperature dependent current density-voltage measurements and impedance spectroscopy are applied.

[1] R.C. Shallcross *et al.*, Adv. Mater. **25**, 469 (2013).

CPP 55.5 Thu 12:00 ZEU 222

Revisiting the Concept of Carrier Heating in Hopping Transport — •Markus Krammer[1], Chris Groves[2], and Karin Zojer[1] — [1]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria — [2]School of Engineering and Computing Science, Durham University, United Kingdom

Charges can be viewed to migrate through amorphous materials like disordered organic semiconductors due to hopping between localised states. This motion is governed by a complex interplay of energetic disorder, electric field, interactions, temperature and other parameters. The concept of carrier heating holds the promise of being able to conveniently predict field-dependent steady state charge carrier densities (SSCCD).[1] The SSCCD can be described with a Fermi Dirac distribution such that the impact of an electric field manifests in an effective temperature; provided that electric field and interactions are weak enough. As the conditions for the validity of this concept are still debated [2], we provide here the exact analytical SSCCD for arbitrary field strengths and low charge carrier densities. We demonstrate that the carrier heating effect originates from a modification of the energetic disorder rather than from an effective temperature. By virtue of numerical Kinetic Monte Carlo simulations, the limits of the effective temperature approximation and the field dependence of the effective temperature are revealed.

[1] B. I. Shklovskii *et al.* in Transport, Correlation and Structural Defects, by H. Fritzsche, World Scientific, Singapore (1990), p. 161

[2] S. D. Baranovskii, Phys. Status Solidi B, 251, 487-525 (2014)

CPP 55.6 Thu 12:15 ZEU 222

On some Fundamentals of Disorder Effects in Organic Semiconductors — •Frank Ortmann[1], Michel Panhans[1], Andreas Lücke[2], Johannes Benduhn[3], Sebastian Schellhammer[1], Gianaurelio Cuniberti[1], Uwe Gerstmann[2], Koen Vandewal[3], and Wolf-Gero Schmidt[2] — [1]Institute for Materials Science, Dresden Center for Computational Material Science and Center for Advancing Electronics Dresden, TU Dresden — [2]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn — [3]Dresden Integrated Center for Applied Physics and Photonic Materials, TU Dresden

Disorder is ubiquitous in Organic Semiconductors but its quantification is rather difficult and depends on the measurement technique. In addition to its magnitude, an open question is if dynamic (thermal) and static disorders behave similar. We show examples of our recent research that shed light on the influence of a static theoretical treatment of vibrational dynamics in transport but also on the possibility of reducing thermal disorder by quantization.

CPP 55.7 Thu 12:30 ZEU 222

Charge Transport in Rubrene Crystals: Dynamic Disorder and Polarons — •Michel Panhans[1], Desanka Boskovic[2], Pablo Ordejòn[2,3], and Frank Ortmann[1] — [1]Institute for Material Science, Dresden Center for Computational Material Science and Center for Advancing Electronics Dresden, TU Dresden — [2]ICN2 - Institut Catala de Nanociencia i Nanotecnologia, Barcelona — [3]CSIC - Consejo Superior de Investigaciones Cientificas, Barcelona

The understanding of charge transport in small-molecule organic semiconductors remains a challenge despite various experimental and theoretical studies in recent years. This is mainly because transport phenomena in organic semiconductors are strongly influenced by vibrations and disorder effects (such as traps, dopants, structural disorder, etc.).

We investigate the temperature dependent p-type charge transport in rubrene crystals including the electron-phonon interaction. This interaction can be either described in terms of vibrational disorder or polaronic effects with different implications for the temperature dependent carrier mobility. We present a new mixed approach with an empirical phonon cutoff energy to study the transition from a semiclassical to a quantum description of electron-phonon interaction.

CPP 55.8 Thu 12:45 ZEU 222

Impact of Polaron Delocalization on Electrical Transport in Conjugated Polymers — Robert Steyrleuthner, Felix Kraffert, and •Jan Behrends — Berlin Joint EPR Lab, Fachbereich Physik, Freie Universität Berlin, Germany

The degree of charge delocalization strongly influences the transport properties of organic semiconductors. However, accurately determining the spatial extension of polaron wave functions remains a challenge. Using electron nuclear double resonance (ENDOR) spectroscopy for measuring the hyperfine coupling between photogenerated polarons and bound nuclear spins, we investigate the delocalization of holes in the semicrystalline conjugated polymer PBTTT (Poly[2,5-bis(3-hexadecylthiophen-2-yl)thieno[3,2-b]thiophene]). An extrapolation of the corresponding oligomer spectra reveals that charges tend to delocalize over 4.0 to 4.8 nm with delocalization strongly dependent on molecular order and crystallinity of the PBTTT polymer thin films.[1]

We further use ENDOR spectroscopy to measure the charge delocalization for a number of conjugated polymers with applications in optoelectronic devices. The results are compared to charge carrier mobilities obtained from time-of-flight measurements, and a correlation between polaron extension and carrier mobility will be discussed.

[1] R. Steyrleuthner, Y. Zhang, L. Zhang, F. Kraffert, B.P. Cherniawski, R. Bittl, A.L. Briseno, J.-L. Bredas and J. Behrends, Phys. Chem. Chem. Phys., 2016, DOI: 10.1039/c6cp07485e

CPP 56: Hydrogels and Microgels I

Time: Thursday 10:15–13:00 Location: ZEU 260

Invited Talk CPP 56.1 Thu 10:15 ZEU 260

Functional microgels: simple matter where complexity matters — •Walter Richtering — RWTH Aachen University, Aachen, Germany, EU

Microgels are macromolecular networks swollen by the solvent they are dissolved in. They are unique systems that are distinctly different from common colloids, such as, e.g., rigid nanoparticles, flexible macromolecules, micelles or vesicles. When swollen, they are soft and have a fuzzy surface with dangling chains and the presence of cross-links provides structural integrity - in contrast to linear and (hyper-) branched polymers. Obviously, the cross-linker content will allow controlling whether microgels behave more ”colloidal” or ”macromolecular”. Finally, microgels reveal interface activity without being amphiphilic. The combination of being soft and porous while still having a stable structure through the cross-linked network allows for the possibility to introduce chemical functionality at different positions. The architectural diversity and compartmentalization of reactive groups enable thus short-range coexistence of otherwise instable combinations of chemical reactivity. The capability of microgels to adjust both their shape and volume in response to external stimuli provides the opportunity to reversibly tune their physico-chemical properties. From a physics point of view, microgels are particularly intriguing and challenging, since their intra-particle properties are intimately linked to their inter-particle behavior.

CPP 56.2 Thu 10:45 ZEU 260

Responsive polymer hydrogels: physical gelling through polyion complexation — Margarita A. Dyakonova[1], Anatoly V. Berezkin[1], Nicoletta Stavrouli[2], Maria T. Popescu[2], Constantinos Tsitsilianis[2], and •Christine M. Papadakis[1] — [1]Technische Universität München, Physik-Department, Fachgebiet Physik weicher Materie, Garching, Germany — [2]University of Patras, Department of Chemical Engineering, Greece

Responsive polymer-based hydrogels may be formed through association of oppositely charged polyion segments [1]. Network formation is due to charged chains which physically crosslink by ion pair formation arising from intermolecular polyionic complexation of oppositely charged repeating units.

We present results from dynamic mechanical measurements, small-angle neutron scattering and computer simulations on hydrogels formed by triblock copolymers bearing oppositely charged blocks (poly(acrylic acid) and quaternized poly(2-vinylpyridine)) [2]. Due to the weak nature of the involved polyions, these hydrogels respond strongly to pH and to the presence of salt.

1. C. Tsitsilianis, C.M. Papadakis, *Gels*, submitted.
2. Dyakonova M. et al., *Macromolecules* **47**, 7561 (2014) and **48**, 8177 (2015).

CPP 56.3 Thu 11:00 ZEU 260

Cell-free protein synthesis and enzymatic cascades in polymer microgels — •Julian Thiele — Leibniz-Institut für Polymerforschung Dresden e.V., Leibniz Research Cluster, Germany

Microfluidic flow cells provide excellent control over the formation of microemulsions, which are widely applied as templates for the fabrication of hydrogel microparticles with defined physicochemical properties and mechanics. The Leibniz Research Cluster group at IPF Dresden utilizes this knowledge to develop biocompatible hydrogel particles as cell-like experimental platform for cell-free biotechnology. Here, spatial organization and confinement of reagents can be easily varied, which directly influence diffusion rates and binding constants, as shown in microgel-based cell-free protein synthesis (Hansen et al. ChemBioChem 2016, 17, 228). Currently, we are extending the application of microfluidically prepared microgels as host for cell-free biosyntheses towards the design of polyketide building blocks in enzymatic cascades.

CPP 56.4 Thu 11:15 ZEU 260

Phase behaviour of PNIPMAM in dependence on temperature and pressure — •Kora-Lee Claude[1], Bart-Jan Niebuur[1], Dionysia Aravopoulou[2], Viet Hildebrand[4], André Laschewsky[4], Apostolos Kyritsis[2], Peter Müller-Buschbaum[1], Alfons Schulte[3], and Christine M. Papadakis[1] — [1]Technische Universität München, Physik-Department, Physik weicher Materie/Lehrstuhl für funktionelle Materialien, Garching, Germany — [2]National Technical University of Athens, Physics Department, Athens, Greece — [3]University of Central Florida, Department of Physics and College of Optics & Photonics, Orlando, U.S.A. — [4]Universität Potsdam and Fraunhofer Institute for Applied Polymer Research, Potsdam-Golm, Germany

Poly(N-isopropylmethacrylamide) (PNIPMAM) is a thermoresponsive polymer which differs from the well-known PNIPAM by having an additional methyl group attached to the vinyl backbone. Thus, it may be expected to be more hydrophobic, however, its cloud point at 42°C is about 10°C higher.

In order to gain more information on the phase behaviour of PNIPMAM in dependence on temperature, pressure and concentration, we investigated the transition by DSC, the structural behaviour by temperature-resolved SANS and mapped out the pressure-dependent phase diagram using turbidimetry.

It seems that the additional methyl group stabilizes the one-phase region, even at higher pressures, which could be explained by steric hindrance.

15 min break

CPP 56.5 Thu 11:45 ZEU 260

Superresolved fluorescence microscopy to gain structural insights into microgels and other soft matter systems — •Dominik Wöll, Alex Oppermann, Arjan Gelissen, Oleksii Nevskyi, and Walter Richtering — Institute of Physical Chemistry, RWTH Aachen University, Germany

The elucidation of the structure of compartimentalized microgels and microgel structures is challenging since they do not possess strong contrast for electron microscopy, and since classical fluorescence microscopy fails due to the fact that their structures are significantly smaller than the diffraction limit of optical light. However, modern superresolved fluorescence microscopy methods such as dSTORM (direct stochastic optical reconstruction microscopy) reach resolutions down to 10-30 nm and, therefore, are highly suited to fill this gap of structural *in situ* imaging. In this contribution, the success of these methods to visualize microgels and other soft matter systems and their application in determining the spatial distribution of implemented functionalities will be demonstrated.

CPP 56.6 Thu 12:00 ZEU 260

Modeling of Polyelectrolyte Gels in Equilibrium with Salt Solutions — Tobias Richter[1], Peter Košovan[2], Jonas Landsgesell[1], and •Christian Holm[1] — [1]University of Stuttgart, Germany — [2]Charles University in Prague, Czech Republic

We use hybrid molecular dynamics/Monte Carlo simulations and coarse-grained polymer models to study the swelling of polyelectrolyte gels in salt solutions. Besides existing industrial applications, such gels have been recently proposed as a promising agent for water desalination. We employ the semi-grand canonical ensemble to investigate partitioning of the salt between the bulk solution and the gel, and the salt-induced de-swelling of the gels under free swelling equilibrium and under compression. We compare our simulation data to the analytic model of Katchalsky and Michaeli which captures the deviations in the ion partitioning from the simple Donnan approximation fairly well [1]. We modify the model by replacing the Gaussian elasticity with the Langevin function for finite extensibility and obtain nearly quantitative agreement between theory and simulations both for the swelling ratio and for the partitioning of salt, across the whole range of studied gel parameters and salt concentrations. The modified model provides a very good description of swelling of polyelectrolyte gels in salt solutions for charge densities up to a Manning parameter of one half. We use this improved model to construct a simple desalination cycle and to calculate the corresponding work to desalinate sea water to potable water. [1] P. Kosovan, T. Richter, C. Holm, Macromolecules 48, 7698-7708 (2015).

CPP 56.7 Thu 12:15 ZEU 260

Structure and Dynamics of highly concentrated PNIPAm microgels. — •Lara Frenzel[1,2], Felix Lehmkühler[1,2], Michael Höltig[1], and Gerhard Grübel[1,2] — [1]DESY, Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, CUI, Hamburg, Germany

Poly (N-isopropylacrylamide) (PNIPAm) is a stimuli responsive crosslinked microgel with a coil-to-globule transition at a lower critical solution temperature (LCST) in water around 32°C, which results in a rapid collapse of the particle radius by increasing the temperature. With this volume phase transition PNIPAm is both applicable in technical as well as medical fields. Furthermore, it became a frequently examined system in research such as a model to study the specific phase behavior of soft colloids. Via x-ray photon correlation spectroscopy (XPCS) we investigate the change in structure and dynamics of PNIPAm microgels at high concentrations around the LCST. Thereby highly brilliant x-rays from the coherence beamline P10 at PETRA III have been used in the XPCS study. Since the swollen microgel shows a low refractive index difference compared to water we studied both pure PNIPAm as well as silica-PNIPAm core-shell systems.

CPP 56.8 Thu 12:30 ZEU 260

A mesoscale hydrodynamic simulation study of polymer dynamics in responsive microgels — •Ali Ghavami, Hideki Kobayashi, and Roland G. Winkler — Institute for Advanced Simulation, Forschungszentrum Juelich GmbH, 52425 Juelich, Germany

We analyze the internal polymer dynamics in microgel systems under different swelling conditions. A microgel particle consists of tetrafunctionally crosslinked linear polymers in solution, which undergoes conformational changes in response to the external stimuli. Here, a broad range of microgel sizes, extending from hydrophobically collapsed to charged swollen particles, are considered and hydrodynamic interactions are accounted through multiparticle collision dynamics method.The polymer dynamics is analyzed in terms of the monomer mean square displacement and the intermediate scattering functions. For microgels in good solvent, the scattering function decays in a stretched-exponential manner, with a decay rate exhibiting a crossover from a collective diffusive-like dynamics at low wavenumbers to a hydrodynamic-dominated dynamics at larger wavenumbers. There is little difference between the intermediate scattering functions of microgels under good solvent conditions and strongly swollen gels, but strongly collapsed gels exhibit a faster decay at short times as the hydrodynamic interactions become screened. In addition, we present results for the dynamics of the crosslinks, which exhibit an unexpected, semiflexible polymer-like dynamics.

CPP 56.9 Thu 12:45 ZEU 260

Polymer dynamics within soft confinement — •Björn Kuttich and Bernd Stühn — Institut für Festkörperphysik, Technische Universität Darmstadt, D-64289, Germany

Microemulsions in the droplet phase are a well suited system to provide a three dimensional soft confining geometry on the length scale of several nano metres. Due to the softness of the confinement molecules which are introduced into the microemulsion droplets will change structural and dynamical properties of the confinement. In case of water in oil microemulsions stabilised by the an-ionic surfactant AOT we studied these changes for the case of the water soluble polymer poly(ethylene oxide) (PEO) enclosed in droplets of different sizes.[1]

Furthermore, structure and dynamics of the confined polymer PEO, are investigated by small angle neutron scattering (SANS) and neutron spin echo spectroscopy (NSE). The SANS show a significant increase of the polymer's radius of gyration, which is related to an attractive interaction between PEO and the AOT head groups. Furthermore the internal correlations of the polymer change to that of a collapsed polymer chain.

For the NSE data the effective diffusion coefficient was investigated. On length scales larger than the droplet size pure droplet diffusion is observed. The polymer is confined to the extent of the droplet. On smaller length scales, thus at larger q values dynamics show a significantly increased effective diffusion coefficient due to the polymer dynamics.

[1] B. Kuttich et al., J. Chem. Phys. **145**, 164904 (2016)

CPP 57: Thin Films, Nanostructures and Nanoparticles I

Time: Thursday 10:15–13:00 Location: ZEU 114

CPP 57.1 Thu 10:15 ZEU 114

Nanostructured diblock copolymers as templates for metal sputter deposition — •Marc Gensch[1,2], Björn Beyersdorff[1], Wiebke Ohm[1], Matthias Schwartzkopf[1], Calvin Brett[1,2], Deniza Chekrygina[2], Pallavi Pandit[1], Andreas Stierle[1,2], and Stephan Roth[1,3] — [1]DESY, Notkestr. 85, D-22607 Hamburg — [2]University of Hamburg, Luruper Chaussee 149, D-22761 Hamburg — [3]KTH, Teknikringen 56-58, SE-100 44 Stockholm

Nanostructured polymer metal composites demonstrate great perspective for flexible electronic and plasmonic applications [1]. Therefore, the growth kinetics and optical properties for silver deposition on co- and homopolymers were characterized by GISAXS, specular reflectance spectroscopy (UVVis), AFM and resistivity measurements. As substrates, solvent annealed PS-b-PMMA diblock copolymers of different molecular weights and their corresponding homopolymers were used. Thus, the influence of the block length and the diblock domains could be investigated. The study reveals the selective wetting of silver on one of the blocks from the copolymer thin films. The silver layers show a clear plasmon resonance. GISAXS measurements indicate a difference in the embedding of silver clusters depending on the polymer substrate. [1] S. V. Roth et al., ACS Appl. Mater. Interfaces 7, 12470 (2015).

CPP 57.2 Thu 10:30 ZEU 114

***In situ* GISAXS of gyroid terpolymer films during selective solvent annealing** — James A. Dolan[1], Karolina Korzeb[2], Raphael Dehmel[1], Bodo D. Wilts[2], Karl C. Gödel[1], Morgan Stefik[3], Ulrich Wiesner[3], Timothy D. Wilkinson[1], Jeremy J. Baumberg[1], Ullrich Steiner[2], and •Ilja Gunkel[2] — [1]University of Cambridge, Cambridge, UK — [2]Adolphe Merkle Institute, Fribourg, CH — [3]Cornell University, Ithaca, NY, USA

Solvent annealing is an effective means to generate order in polymer systems. When solvent enters a film, the resultant plasticization drastically increases the mobility of the polymer chains. Annealing diblock copolymers in selective solvents has already been shown to induce morphological transitions from spheres to cylinders, gyroids, or lamellae. However, for the next more complicated family of linear block copolymers, triblock terpolymers, the morphological effect of selective solvent annealing is not well understood. Therefore, we present the results of *in situ* GISAXS during selective solvent annealing of gyroid-forming polyisoprene-*b*-polystyrene-*b*-poly(ethylene oxide) triblock terpolymer films. The selectivity was adjusted by using mixed vapor ratios of tetrahydrofuran and methanol. Distinct from diblock copolymers, we found that irrespective of the solvent vapor ratios used for annealing, the gyroid morphology remained. However, the selectivity of the solvent did either increase or decrease the unit cell size of the gyroid in both swollen and dried films.

CPP 57.3 Thu 10:45 ZEU 114

Selective metal deposition on block copolymer nanotemplates: A new perspective — •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

The characteristic metal affinity towards one block of self-assembled block copolymer (BC) templates plays an essential role to fabricate highly-order and well-defined metal nanopatterns. Deposition of inert metal atoms on several BC nanotemplates shows an extreme selectivity towards the glassy polymer nanodomain [1]. An explanation based on a difference in the metal-polymer interaction energy cannot adequately explain such extreme affinity. To better investigate this phenomenon, RF magnetron sputtering system was used to deposit gold metal in its atomic state on glassy poly(methylmethacrylate) and soft poly(ethylhexylacrylate) amorphous homopolymers as well as the corresponding statistical copolymer P(EHA-stat-MMA). At time resolution of 15 milliseconds, the nucleation/growth kinetics of gold nanoparticles on these polymer films was monitored using in situ grazing incidence small angle X-ray scattering (GISAXS). The coalescence behavior of the inert metal is mainly dominated by an improved atom mobility within the glassy polymers. This study on polymer thin films provides a new perspective into the long-time debated high selectivity characteristics of metals towards one block of BC based nanotemplates. [1]S. V. Roth et al., ACS Appl Mater Inter 2015, 7, 12470.

CPP 57.4 Thu 11:00 ZEU 114

In situ GISAXS study of Aluminum thin film growth on PS-b-PMMA and its constituent homopolymers — Björn Beyersdorff[1], •Matthias Schwartzkopf[1], Wiebke Ohm[1], Alexander Hinz[2], Thomas Strunskus[2], Oleksandr Polonskyi[2], Franz Faupel[2], Volker Körstgens[3], Franzika Löhrer[3], Peter Müller-Buschbaum[3], and Stephan V. Roth[1,4] — [1]Deutsches Elektronen-Synchrotron DESY — [2]Christian-Albrechts-Universität zu Kiel — [3]Technische Universität München — [4]KTH Royal Institute of Technology

Installation of nanostructured metal films with tailored optical properties is of high importance in many areas of modern science and technology. Aluminum (Al) nanostructures for instance are very promising for surface-enhanced Raman Scattering (SERS) due to their wide tuneability of the plasmon resonance [1]. When depositing metal by sputter deposition on a nanostructured diblock copolymer substrate, a different adatom mobility on the two polymer blocks leads to selective wetting of one block and thus to an imitation of the polymer structure by the metal atoms [2,3]. We report on the sputter deposition of Al on a PS-b-PMMA diblock copolymer thin film and its two constituent homopolymers PS and PMMA by means of grazing incidence small-angle X-ray scattering (GISAXS). Cluster growth kinetics on the diblock and the homopolymer films is analyzed and compared to ex situ samples investigated by AFM. [1] Gérard et al, J. Phys. D: Appl. Phys., 48, 184001 (2015), [2] Lopes et al, Nature 414, 735 (2001), [3] Roth et al, ACS Appl. Mater. Interfaces 7 (23), 12470 (2015)

CPP 57.5 Thu 11:15 ZEU 114

Structural evolution of gold-teflon nanocomposite multilayer structure — •Pallavi Pandit[1], Ajay Gupta[2], Sigrid Bernstorff[3], Matthias Schwartzkopf[1], Deniza Chekrygina[4], and Stephan Roth[1] — [1]DESY, Notkestr. 85, D-22607 Hamburg — [2]Amity University, 201313 Noida India — [3]Elettra, SS 14, I-34149 Basovizza Trieste — [4]UHH, Lurup. chaus. 149, D-22761 Hamburg

The combination of metal nanoparticles in polymer metrics has gained sustained research interest as their fine control of size and shape leads to the fabrication of materials with novel electronic, magnetic and catalytic properties. This offers some level of controllable performance. Thermal annealing as well can artificially modify the morphology of embedded metal nanoparticles. In this study the structural evolution of gold/PTFE multilayer nanocomposite has been studied using in-situ temperature dependent Grazing incidence Small and wide angle X-ray scattering. Nanoparticles exhibited a lognormal size distribution in multilayer structure. A rather well defined inter-particle correlation is observed in lateral and vertical direction. Linear dependence of the size of nanoparticles on square root of annealing time suggests a diffusion control growth of nanoparticles. After annealing at 573 K the nanoparticles distribution become isotropic in both the directions. UV-Vis reflectance spectroscopy has been used to study the Surface Plasmon Resonance of gold nanoparticles. The SPR frequency exhibits a systematic variation with gold content as well as with thermal annealing.

15 min break

CPP 57.6 Thu 11:45 ZEU 114

Printed nanostructured polymer films embedded with magnetic nanoparticles — •Senlin Xia[1], Ezzeldin Metwalli[1], Matthias Opel[2], Paul A. Staniec[3], Eva M. Herzig[4], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching — [3]Beamline I22, Diamond Light Source, Harwell, OX11 0DE, United Kingdom — [4]TU München, Munich School of Engineering, Herzig Group, Lichtenbergstr. 4, 85748 Garching

Nanostructured polymer films containing magnetic nanoparticles (NPs) are promising materials due to their potential applications in the areas of high-density storage and magnetic sensors. Owing to the advantages, like large-scale production and energy saving, printing techniques were employed to fabricate hybrid films composed of maghemite NPs and PS-b-PMMA diblock copolymer (DBC). External magnetic fields were applied during the printing process to guide the NPs within the polymer matrix. The mesoscopic structure of PS-coated maghemite NPs within the DBC films was investigated as a function of the NP concentration using optical microscopy, AFM, SEM and GISAXS. The PS-coated NPs were selectively dispersed in the PS domains of the lamella-structured hybrid films. At high NP concentrations, the coalescence of NPs into large micro-sized metal-oxide wires was observed. The superparamagnetic behavior of the hybrid film was proved using a superconducting quantum interference device magnetometer.

CPP 57.7 Thu 12:00 ZEU 114

vinyl-terminated Au nanotriangles as platform for the fabrication of hybrid Au@pNIPAM particles for improved SERS responses. — Miguel Casado-Rodriguez[1], Christian Kuttner[2], Manuel Lopez-Romero[1], Andreas Fery[2,3], and •Rafael Contreras-Caceres[2] — [1]Universidad de Malaga, Departamento de. Quimica Organica. Facutlad de Ciencias. Universidad de Malaga 29071. Malaga. Spain — [2]Leibniz-Institut fu*r Polymerforschung, Dresden e.V. Hohe Strasse 6, 01069 Dresden, Germany — [3]Physical Chemistry of Polymeric Materials, Technische Universita*t Dresden, 01069 Dresden, Germany

We present a new approach for a water-based seedless synthesis of vinyl-terminated triangular Au nanotriangles. This method enables temperature controllable Au size by using 3-butenoic acid as reducing agent. We initially analyze the influence of the temperature on the particle size. Interestingly, the presence of terminal double bonds on the Au nanotriangle surface (coming from 3BA) is exploited for the fabrication of core@shell hybrid systems by free radical polymerization of N-isopropylacrylamide (AuNT@pNIPAM). Additionally, Au overgrowth using AuNTs@pNIPAM as seeds permits the fabrication of Austars@pNIPAM particles. The SERS enhancement capabilities of these two core*shell hybrids demonstrate that Au cores with tips and high curvature sites produced the highest plasmonic responses.

CPP 57.8 Thu 12:15 ZEU 114

Nanostructure tuning of sputter deposited Al layers on polystyrene using bias voltage — •Stephan V. Roth[1,2], Matthias Schwartzkopf[2], Björn Beyersdorff[2], Calvin Brett[2], Marc Gensch[2], Wiebke Ohm[2], Andre Rothkirch[2], Alexander Hinz[3], Oleksandr Polonskyi[3], Thomas Strunskus[3], Franz Faupel[3], Franziska C. Löhrer[4], Volker Körstgens[4], Adrian Haussmann[4], Lorenz Biessmann[4], and Peter Müller-Buschbaum[4] — [1]KTH, Teknikringen 56-58,SE-100 44 Stockholm — [2]DESY, Notkestr. 85, D-22607 Hamburg — [3]CAU, Kaiserstr.2, D-24143 Kiel — [4]TUM, James-Franck-Str. 1, D-85748 Garching

Nanostructuring the polymer-metal interface in thin films is crucial for organic photovoltaics, flexible electronics and sensors. Hence, we investigated in real-time the different growth kinetics of nanostructured Aluminum layers on polystyrene thin film substrates during DC sputter deposition at applied bias voltages from 0V to -400V and at industrial coating rates. Using grazing incidence X-ray scattering and UV-Vis spectroscopy, we were able to directly correlate the crystallinity, the nanogranular structure and the optical properties at all growth stages during in situ sputter deposition at the applied bias voltages. Electron microscopy confirmed a transition in the nanogranular structure at a bias voltage around -300 V from a densely packed via a worm-like transient stage to a large cluster layer. Our results offer a versatile route for fabricating tailored metal arrays, ranging from nanoparticulate layers to full scale electrical contacts.

CPP 57.9 Thu 12:30 ZEU 114

In situ GISAXS analysis of spray deposited biopolymer thin films — Wiebke Ohm[1], Björn Beyersdorff[1], Matthias Schwartzkopf[1], Pallavi Pandit[1], Calvin Brett[1], Marc Gensch[1], Shun Yu[2], Nitesh Mittal[2], Daniel Söderberg[2], and •Stephan Roth[1,2] — [1]Deutsches Elektronen-Synchrotron Hamburg, Notkestraße 85, 22607 Hamburg — [2]KTH Royal Institute of Technology, Department of Fibre and Polymer Technology, Teknikringen 56-58, SE-100 44 Stockholm, Sweden

Flexible biopolymer substrates based on cellulose nanofibrils (CNFs) are gaining increasing interest for nanotechnology such as organic electronics or solar cells since they present a renewable and sustainable alternative for synthetic polymers. In view of efficient industrial scalable fabrication, both the controlled arrangement of the CNFs during deposition and the use of industrial compatible deposition processes are essential.

We thus applied air-brush spray deposition of aqueous dispersions of CNF/water as a versatile deposition technique for preparing of cellulose thin films [1]. In situ grazing incidence small angle x-ray scattering (GISAXS) and atomic force microscopy measurements revealed the inner structure of these cellulose films. The effect of different types of CNFs was explored, enzymatic cellulose as well as TEMPO oxidized cellulose with different surface charges. The influence of different incidence angles of the spray was studied to reveal the impact on ordering of the CNFs. [1] Roth, J. Phys.: Condens. Matter 28, 403003(2016)

CPP 57.10 Thu 12:45 ZEU 114

An in-situ STXM approach to understand soft x-ray induced chemical modification in polymers — •Markus Meyer[1], Andreas Späth[1], Benjamin Watts[2], and Rainer H. Fink[1] — [1]Friedrich-Alexander Universität Erlangen-Nürnberg, Physikalische Chemie II, Erlangen, Germany — [2]SwissLight Source (SLS), Paul Scherrer Institut, Villigen, Switzerland

Certain binding motifs in organic molecules are very sensitive to UV or XUV irradiation which induces severe chemical modifications. Scanning transmission x-ray microspectroscopy (STXM) was used to follow the evolution of effects like mass loss (due to bond rupture) and chemical changes of sample in an all but in-situ fashion. In our studies we investigated carbonyl group containing ultrathin free-standing films of PMMA, PLA and polycarbonate. The aim is a comprehensive study on x-ray induced chemical modification of the target for resonant and non-resonant excitations. It is found that the cleavage of chemical bonds does not follow a defined reaction pathway, thus directly leading to the formation of new C=C double bonds. In contrary, our studies provide clear evidence of small molecule fragments leaving the sample, thereby changing the chemical nature of the pristine material. This process is accompanied by deposition of residual gas onto the sample of interest as an unavoidable secondary process. Theoretical considerations are applied in a simulation and are able to retrace and to confirm the findings of the in-situ STXM analysis going well beyond recent publications [1]. [1] Leontowich, A. et al, JElectronSpectrosc, 58-64, 206, 2016

CPP 58: Fluids and Interfaces II

Time: Thursday 10:15–12:45 Location: ZEU 255

CPP 58.1 Thu 10:15 ZEU 255

Elastic capsules at liquid-liquid interfaces — •Jonas Hegemann[1], Horst-Holger Boltz[2], and Jan Kierfeld[1] — [1]TU Dortmund, 44221 Dortmund, Germany — [2]Georg-August-Universität Göttingen, 37077 Göttingen, Germany

We investigate capsules consisting of a hollow spherical shell filled with an incompressible liquid. We consider shells made from isotropic and thin materials with Hookean bending and stretching elasticity. When adsorbing to a liquid-liquid interface, initially spherical capsules undergo equatorial expansion due to isotropic in-plane tension and become discus-shaped. During spreading within the liquid-liquid interface, the adsorption energy increases significantly leading to mechanical stabilization of the interface. The full range of shapes is bounded between the spherical rest shape and a liquid lense, whose shape is solely determined by balance between the set of surface tensions and pressure differences. The intermediate regime can be explored in terms of the shell's elastic moduli. By use of non-linear elastic shell theory, we calculate capsule shapes at liquid-liquid interfaces and provide a method, which allows for estimating the elastic moduli from experimental setups.

CPP 58.2 Thu 10:30 ZEU 255

Structuring of micro particle assemblies at the solid liquid interface by light driven diffusioosmosis — •David Feldmann[1], Salim Maduar[2], Olga I. Vinogradova[2,3,4], and Svetlana Santer[1] — [1]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany — [2]A.N. Frumkin Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, 119071 Moscow, Russia — [3]Department of Physics, M. V. Lomonosov Moscow State University, 119991 Moscow, Russia — [4]DWI-Leibniz Institute for Interactive Materials, RWTH Aachen, 52056 Aachen, Germany

Light-induced diffusioosmotic flows can be used to manipulate and structure particle assemblies at the solid liquid interface.[1] The main player is an azobenzene containing cationic surfactant. Azobenzene switches from a trans to a cis state under UV and back under visible light or by thermal relaxation. A particle-surfactant dispersion is pipetted onto a substrate and placed under a microscope, in which two lasers (UV, green) are coupled. Surfactant adsorbs to the surface, depending on isomer and surface properties, and creates an electrical double layer(EDL). Local irradiation induces a gradient in surfactant concentration creating a diffusioosmotic flow in the EDL, which drags particles on the surface either away (UV) or to (green) the laser spot, with velocities around 1μm/s. With these flows we clean, gather, and structure particles assemblies on flat surfaces or direct particles along patterned surfaces.[1]Feldmann, D. et al. Sci. Rep. 6, 36443; doi: 10.1038/srep36443 (2016).

CPP 58.3 Thu 10:45 ZEU 255

Deriving interaction potentials to simulate self-assembly of graphene particles at the oil-water interface — •Vikram Reddy Ardham and Frédéric Leroy — Eduard-Zintl-Institut für Anorganische und Physikalische Chemie,TU Darmstadt

High interfacial tension between immiscible liquids can provide necessary driving force for the self-assembly of nano-particles at the interface. Particularly, water-oil interfaces have been exploited to synthesize networks of highly inter-connected graphene flakes of only up to a few layers thick. To simulate and study these systems, we derive coarse-grained (CG) force-fields for particle-liquid interactions. CG potentials derived using the standard approaches often give rise to free energies far from the reference system and might not lead to any self-assembly at the interface, since the entire process is possible only within a narrow window of interfacial free energies determined by the wetting coefficient (ω) [Polym. Bull. 1991, 25 (2), 265-271]. Therefore, we derive CG particle-liquid interaction potentials [J. Chem. Phys. 2015, 143 (24)] to get the right free energy balance and therefore the right 'ω'. The derived coarse-grained potentials provide accelerated dynamics of up to a few orders of magnitude without losing the thermodynamic or much of the structural information. Further, we illustrate the applicability of method by simulating a relatively large water-oil interface with graphene particles forming an inter-connected network using the derived coarse-grain model. The method might find applications in multi-scale modeling of polymer nano-composites where a great deal of solid-liquid interface is to be modelled accurately.

Invited Talk CPP 58.4 Thu 11:00 ZEU 255

Molecular Scale Structure of Ionic Liquid Surfaces — •Markus Mezger — Institut für Physik, Johannes Gutenberg-Universität Mainz — Max-Planck-Institut für Polymerforschung, Mainz

Ionic Liquids (ILs) are promising candidates in a variety of applications such as heterogeneous catalysis. For understanding and optimizing the transport properties of reactants and products at IL interfaces, knowledge of their interfacial structure on the molecular length scale is highly desirable. Our x-ray reflectivity (XRR) studies of IL based electrolytes provide density profiles across liquid/vapor interfaces with sub-nanometer resolution. Depending on the molecular architecture of anions and cations, we observe the pinning of bulk correlations at the surface and surface induced smectic order. As model system for blends containing dielectric solvents, we studied the near surface structure of an alkane containing IL. Analysis of the experimental data revealed surface segregation of the alkanes that induce ordered structures, affecting the interfacial ion profiles over a length scale up to 50 nm.
M. Mezger et al., Proc. Natl. Acad. Sci. USA 110, 3733 (2013).
M. Mezger, et al., J. Chem. Phys. 142, 164707 (2015).

15 min break

CPP 58.5 Thu 11:45 ZEU 255

Influence of surface charge on interfacial water arrangement — •Lisa Dreier[1,2], Ellen Backus[1], and Mischa Bonn[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Graduate School Materials Science in Mainz, Mainz, Germany

For a charged surface in contact with an aqueous solution, the decay of the electric potential towards bulk liquid has been described by various models for the electric double layer. Usually, the electrostatic behavior of charged lipid-water interfaces is interpreted in the same way, even though the charge at these interfaces is highly localized. Here, we test experimentally to what extent electric double layer models for solid-liquid interfaces are applicable for lipid-water interfaces, especially very close to the surface in these systems. We study the water organization at the water-lipid interface using the non-linear optical spectroscopy vibrational Sum-Frequency Generation (SFG). Requiring that symmetry is broken, SFG is highly surface-selective, and provides the vibrational spectrum of specifically interfacial molecules; the SFG intensity can be related to the degree of interfacial water alignment. The charge carried by the interface orients interfacial water molecules. By mixing positively and negatively charged lipids, we can vary the surface charge at constant area per lipid molecule. Surprisingly, one can change the lipid layer composition, and thus the surface charge, dramatically without substantially influencing the arrangement of the water molecules. The SFG intensity, and thus the water orientation, responds in a remarkably strong nonlinear fashion to changes in the surface charge.

CPP 58.6 Thu 12:00 ZEU 255

Hydrogen and Electric Power Generation from Liquid Microjets: Design Principles for Optimizing Conversion Efficiency — •Nadine Schwierz, Royce K. Lam, Phillip L. Geissler, and Richard J. Saykally — Department of Chemistry, University of California, Berkeley, California 94720, United States

Liquid water microjets have been successfully employed for both electrical power generation and gaseous hydrogen production, but the demonstrated efficiencies have been low. Here, we employ a combination of a modified Poisson Boltzmann description, continuum hydrodynamic equations, and microjet electrokinetic experiments to gain detailed insight into the origin of the streaming currents produced in pure water. We identify the contributions to the streaming current from specific ion adsorption at the solid/liquid interface and from long-ranged electrostatic interactions, finding that the portion originating from the latter dominate at charged surfaces. The detailed understanding afforded by theory and the close agreement with experimental results elucidates design principles for optimizing hydrogen production and power generation. Changing the sign of the surface charge density through targeted use of surface coatings via silanization switches the primary charge carrier between hydronium and hydroxide and therefore switches the corresponding production of molecular hydrogen to oxygen at the target electrode. Moreover, hydrophobic surface coatings reduce dissipation due to fluid/solid friction, thereby increasing the conversion efficiency.

CPP 58.7 Thu 12:15 ZEU 255

Bridging phases: Permittivity studies at interfaces for ITIES catalysts — •David Egger, Zhu Liu, Christoph Scheurer, and Karsten Reuter — Technische Universität München, Germany

"Interfaces between Two Immiscible Electrolyte Solutions" (ITIES) - typically, between an aqueous and an organic solvent (OS) - have recently emerged as promising environments for electrocatalytic processes. Amphiphilic MoS_2-based complexes at ITIES are of particular interest for photocatalytic water splitting. It is expected that an appropriate bandgap engineering could lead to a further boost in quantum efficiency that renders ITIES-based solar hydrogen generation technologically viable. Approaching this context from the perspective of predictive-quality first-principles electronic structure calculations a major challenge rests in the accurate, yet efficient representation of the effect of the ITIES environment on the catalytic complex. To this end, we present a tailored implicit solvation approach, in which the liquid-liquid interface surrounding the catalytic complex is coarse-grained to a spatially varying dielectric medium. Across interfaces, this transition function exhibits a strong electrostatic correlation, as recently shown for soft polar interfaces in aqueous environment [1]. Based on classical molecular dynamics simulations we present an approach to model consistent permittivity transition functions across the relevant phase interfaces of the ITIES system. We discuss first numerical results for the topologically significant interfaces of MoS_2-water, MoS_2-OS, as well as the triphase point MoS_2-water-OS. [1] A. Schlaich, E.W. Knapp, and R.R. Netz, Phys. Rev. Lett. **117**, 048001 (2016).

CPP 58.8 Thu 12:30 ZEU 255

Dielectric Permittivity Tensor of the Intrinsic Liquid-Liquid Interface — •Zhu Liu, Karsten Reuter, and Christoph Scheurer — Technische Universität München, Germany

As an important continuum response property of liquids at a shared interface, the dielectric permittivity tensor sensitively reflects the unique microscopic characteristics in the interfacial region. Simulations of interfacial dielectric properties have so far mostly considered the case of confined liquids at a rigid solid/mobile liquid interface [1]. Liquid/liquid interfaces are instead known to be intrinsically fluxional in nature [2,3]. This requires statistical procedures devised to analyze molecular dynamics simulations for the computation of the dielectric tensor fields to be adjusted accordingly. We present a novel approach to this problem which yields dielectric profiles with features of similar sharpness as for the solid/liquid case – if the statistical analysis is consistently referenced to the instantaneous liquid/liquid interface. In contrast, simple statistical analyses based on an average interface definition only result in broadened featureless dielectric profiles across the interface region. Numerical results will be presented for the prototypical 1,2-dichloroethane/water liquid/liquid interface, using a reparametrized force-field for the organic solvent.

[1] D.J. Bonthuis, *et al.*, Langmuir **28**, 7679 (2012).
[2] V. Privman, Int. J. Mod. Phys. C **3**, 857 (2012).
[3] A. Schlaich, *et al.*, Phys. Rev. Lett. **117**, 048001 (2016).

CPP 59: Focus: Static and Dynamic Disorder Phenomena on the Transport in Organic Semiconductors II

Time: Thursday 15:00–18:00 Location: ZEU 222

Invited Talk CPP 59.1 Thu 15:00 ZEU 222

Charge transport modeling in disordered molecular semiconductors: from the molecule to the device — Andrea Massé[1], Feilong Liu[1], Pascal Friederich[2], Franz Symalla[2], Velimir Meded[2], Wolfgang Wenzel[2], Reinder Coehoorn[1], and •Peter A. Bobbert[1] — [1]Department of Applied Physics, Technische Universiteit Eindhoven, Eindhoven, The Netherlands — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany

The modeling of charge transport in disordered organic molecular semiconductors has been hampered up to now by the huge difference between the molecular scale and the device scale at which the transport is studied experimentally. Here, we employ a multi-scale approach in which microscopic information based on ab initio calculations of the morphology, energy disorder, reorganization energies, and charge transfer integrals is stochastically expanded to a scale that allows charge transport calculations at the device scale. We demonstrate the approach for electron and hole transport in a few important molecular semiconductors. For hole-only α-NPD devices, we find a remarkable agreement between predicted and measured temperature-dependent current-voltage and impedance spectroscopy characteristics, without the need to adjust a single parameter. We study the effects of spatial energy correlations and superexchange on charge transport and find that the latter can significantly increase the conductance of host-guest systems used in the emission layers of organic light-emitting diodes.

Invited Talk CPP 59.2 Thu 15:30 ZEU 222

Charge transport in high mobility molecular semiconductors — •Henning Sirringhaus — Cavendish Laboratory, University of Cambridge, Cambridge, UK

Over recent years there has been tremendous progress in developing low-temperature processible organic semiconductors that provide high charge carrier mobilities for both n-type and p-type device operation, good operational stability and other functionalities such as efficient electroluminescene, sensing or memory functions for a variety of applications. Here we are interested in understanding the charge transport physics of high mobility conjugated polymers and molecular single crystals and the relationship between molecular structure, solid-state microstructure and charge transport. In this presentation we will present our current understanding of the key factors that govern the transport physics and carrier mobilities of these materials.

CPP 59.3 Thu 16:00 ZEU 222

Theory of Thermalization and Recombination in Organic Disordered Semiconductors — •Andreas Hofacker[1], Dieter Neher[2], Koen Vandewal[1], and Karl Leo[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials, Dresden University of Technology, D-01069 Dresden — [2]Institute of Physics and Astronomy, University of Potsdam, D-14469 Potsdam

Charge carrier recombination in organic disordered semiconductors is strongly influenced by thermalization of charge carriers in the density of states (DOS). Measurements of recombination dynamics, conducted under transient or steady-state conditions, can easily be misinterpreted when a detailed understanding of the interplay of thermalization and recombination is missing. To enable adequate measurement analysis, we solve the multiple-trapping problem for recombining charge carriers and analyze it in the transient and steady excitation paradigm for different DOS distributions.

We show that recombination rates measured after pulsed excitation are inherently time-dependent, since recombination gradually slows down as carriers relax in the DOS. When measuring the recombination order after pulsed excitation, this leads to an apparent high-order recombination at short times. As times goes on, the recombination order approaches an asymptotic value. For the Gaussian and the exponential DOS distributions, this asymptotic value equals the recombination order of the equilibrated system under steady excitation. For a more general DOS distribution, the recombination order can also depend on the carrier density, under both transient and steady-state conditions.

CPP 59.4 Thu 16:15 ZEU 222

Dispersive Charge Transport and Recombination in Polymer Solar Cells — •John Love and Dieter Neher — University of Potsdam

Charge transport in organic semiconductors has long been known as governed by hopping through a broad distribution of localized electronic states. Yet, the role of charge relaxation and dispersive charge transport in the steady state operation of organic solar cells, remains highly debated. Here we address this question, of how thermalization determines the dynamics of charge transport and non-geminate recombination, in the TQ1:PCBM system. Via time delayed collection field, a state-of-the-art dynamic charge extraction technique, we are able to experimentally follow the rate of recombination from nanoseconds to microseconds inside of a working device. We show that the recombination indeed shows a pronounced slowing over time, experimentally validating results of previously published Monte Carlo simulations.[1] The steady state recombination rate at open circuit voltage matches well with the nearly fully relaxed charges found at long time scales of the transient experiments suggesting that open circuit, it is relaxed carriers which undergo recombination.

[1] Melianas, A., Pranculis, V., Devizis, A., Gulbinas, V., Inganas, O. and Kemerink, M. (2014), Adv. Funct. Mater., 24: 4507.

15 min break

CPP 59.5 Thu 16:45 ZEU 222

Identifying Charge Transfer States in Polymer:Fullerene Heterojunctions by Their Emission Polarization Anisotropy — Andreas Arndt[1], Marina Gerhard[2], Martin Koch[2], Uli Lemmer[1,3], and •Ian Howard[1,3] — [1]Karlsruhe Institute of Technology (Light Technology Institute), Karlsruhe, Germany — [2]Philipps-Universität Marburg, Marburg, Germany — [3]Karlsruhe Institute of Technology (Institute of Microstructure Technology), Karlsruhe, Germany

It is well understood that the separation of charge carriers from donor:acceptor heterojunctions in organic photovoltaic blends is significantly affected by the distribution of charge-transfer states present at the disordered material interface. Recombination of charge carriers held in charge-transfer states can be emissive, meaning the emission spectrum of the charge-transfer states reveals information about interfacial disorder. However, the assignment of charge-transfer state emssion can be controversial, especially when the offset to low-energy excitonic emission is small. In this contribution, we present the time-resolved photoluminescence (PL) polarization anisotropy of several organic photovoltaic blends. Our results demonstrate that the charge-transfer state emission can be identified with a high degree of certainty by its unique negative polarization anisotropy. The unique negative anisotropy arises due to the significant rotation of the transition dipole moment upon charge-transfer at the donor-acceptor interface.

CPP 59.6 Thu 17:00 ZEU 222

DFT Study on the Intercalation of Fullerenes and AnE-PV Copolymers — •Wichard J. D. Beenken and Chuan-Ding Dong — Technische Universität Ilmenau, Institut für Physik, Germany

Using density functional theory calculations, we studied the order and disorder of poly(p-anthracene-ethynylene)-alt-poly(p-phenylene-vinylene) copolymers (An-E-PV) with two different substitution schemes for straight and branched side-chains [1,2] and their influence on the intercalation with C_{60}. We found that the calculated ordered and intercalated structures are all in good agreement with the experimental XRD data for films made of ternary blends of these two copolymers with PCBM [3]. The conclusions drawn from the calculated crystal structures and the corresponding electronic band structures explain the experimentally observed variations in photocurrent, photoluminescence [3] and electroluminescence yields with the concentration ratio of the two copolymers in the ternary blend with PCBM.

[1] C.-D. Dong, H. Hoppe, and W. J. D. Beenken, *J. Phys. Chem. A* **120**, 3835 (2016); [2] C.-D. Dong and W. J. D. Beenken,*J. Phys. Chem. B* 2016, **120**, 10854 (2016); [3] C. Kästner *et al. J. Mater. Chem. A* **1**, 3961 (2013).

CPP 59.7 Thu 17:15 ZEU 222

Origin of high energy photoluminescence in poly(3-hexylthiophene) films — •Philipp Ehrenreich[1], Daniel Proepper[2], Stefan Jores[1], Alexander Boris[2], and Lukas Schmidt-Mende[1] — [1]Department of Physics, University of Konstanz, POB M 680, Konstanz 78457, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany

A deeper understanding of exciton dynamics in polymer films is crucially important for improving charge generation in organic photovoltaics further. The large number of already existing polymers and unlimited possibilities of designing new materials demands for model systems, to which a comparison is possible. For this purpose, poly(3-hexylthiophene) is commonly used. Nonlinear decay kinetics have been interpreted by means of hot-excitons, torsional relaxation effects or exciton dissociation at amorphous/crystalline interfaces. However, it is often seen that observations vary. This is attributed to structural or energetic differences that depend on processing conditions. Using temperature dependent time-resolved photoluminescence measurements in combination with low temperature ellipsometry, we can show that P3HT is indeed a model system that follows the common diffusion model of excitons. Based on our results we can exclude the existence of hot-exciton emission as well as an impact of torsional relaxation dynamics on exciton decay dynamics.

CPP 59.8 Thu 17:30 ZEU 222

Ambipolar Seebeck coefficients in high-mobility polymers — •Katharina Broch[1,2], Deepak Venkateshvaran[2], Vincent Lemaur[3], Yoann Olivier[3], and Henning Sirringhaus[2] — [1]Cavendish Laboratory, University of Cambridge, JJ Thomson Ave, CB3 0HE Cambridge, UK — [2]Fritz-Haber-Institute of the Max-Planck-Society, Faradayweg 4-6, 14195 Berlin, Germany — [3]3Laboratory for Chemistry of Novel Materials, Université de Mons, 20 Place du Parc, 7000 Mons, Belgium

Ambipolar polymers with high charge carrier mobilities have attracted considerable interest owing to their potential use in state-of-the-art organic electronic devices. For further advances in mobility and device performance, a deeper understanding of the molecular building schemes leading to low energetic disorder and, in turn, high charge carrier mobilities, is vital. It has been shown that the voltage modulated Seebeck coefficient can be an excellent probe of energetic disorder within unipolar polymer field effect transistors (FETs) [1], but due to experimental challenges a measurement of the Seebeck coefficient of electrons and holes in ambipolar polymers was difficult to achieve. Here, we report the simultaneous measurement of the Seebeck coefficients of both charge carrier species in high mobility polymers based on diketopyrrolopyrrole and discuss the origins of their high performance in FETs combining our experimental findings with numerical simulations of the energetic broadening of the density of states.

[1] D. Venkateshvaran et al., Nature 2014, 515, 384-388

CPP 59.9 Thu 17:45 ZEU 222

Asymmetric bodipy end-capped oligomer: A molecular seesaw as a polarization-to-wavelength converter — •Philipp Wilhelm[1], Jakob Schedlbauer[1], Florian Hinderer[2], Sigurd Höger[2], Jan Vogelsang[1], and John M. Lupton[1] — [1]Universität Regensburg, Universitätsstraße 31, 93053 Regensburg, Germany — [2]Universität Bonn, Gerhard-Domagk-Straße 1, 53121 Bonn, Germany

Excitation energy transfer (EET) plays a crucial role for the properties of organic photovoltaic devices. Unfortunately, the microscopic pathways of EET are hard to monitor. We therefore introduce a model system, which consists of a π-conjugated donor oligomer (emitting in the blue wavelength region with λmax=450 nm) and two different acceptor dyes, based on bodipy (boron-dipyrromethene) derivatives and located at each end of the oligomer. One of the bodipy endcap units emits in the green (λmax=515 nm) and the other one in the red (λmax=650 nm) wavelength region. By using this molecule with two competing EET pathways from the oligomer to the asymmetric endcaps, we can learn whether the excitation energy migrates preferentially to the global minimum (i.e. the red dye) or if EET is non-deterministic. By employing single-molecule spectroscopy we can address the following questions: does the EET pathway differ between individual molecules? Is the EET pathway like a "seesaw", dynamically changing between red and green over time? Finally, we looked into the question whether the EET pathway can be influenced externally by changing the polarization of the excitation laser. Indeed, we find that the model system can act as a single-molecule light polarization to wavelength converter.

CPP 60: Focus: Topological Problems in the Physics of Polymers, Biopolymers and Fibers I (joint session BP/CPP, organized by CPP)

Organisers: Raffaello Potestio (MPI Polymer Research, Mainz), Luca Tubiana (University of Vienna), Peter Virnau (Johannes Gutenberg Universität Mainz) and Rudolf Podgornik (University of Ljubljana)

The topological, or knotted, state of long chains influences their physical properties. Mechanical features of polymers and fibers, such as energy dissipation and tensile rupture, are known to be substantially affected by the presence and type of a knot. Entanglements have emerged as relevant players also in the realm of biophysics, as knots have been found in circular DNA as well as in proteins. In the last few decades a great effort has been put in the characterization of the properties of chains featuring a self-entangled topology. A large contribution has been provided in particular by computer simulations of knotted polymers, with a spectrum of different models and systems spanning from ideal chains to atomistic proteins and coarse-grained chromosomes. Furthermore, the advancement of experimental techniques has enabled researchers to construct, handle, and study physical knots, making possible a productive interplay between theory, computer modeling, and experimental validation. The scope of this focus session is to bring together scientists active in the multifaceted field of polymer topology, and foster the exchange of ideas among different areas. In particular, it is our aim to promote the interaction between two communities, polymer science and biophysics, that have insofar manifested a great collaborative potential.

Time: Thursday 15:00–18:00 Location: ZEU 260

Invited Talk CPP 60.1 Thu 15:00 ZEU 260

Polymers in the cell nucleus — •Maria Barbi, Antony Lesage, and Jean-Marc Victor — Laboratoire de physique Theorique de la Matiere Condensee - UPMC - Paris VI - France

Understanding the genome functional architecture and its dynamics is one of the big challenges of systems biology. The three-dimensional arrangement, in the cell nucleus, of the protein-DNA assembly that constitutes chromosomes is expected to be crucial for the regulation of gene expression, hence cell differentiation and cell type setting. The rapid progress of experimental techniques Begins to make it possible to explore these complex structures. I will show how, when used in connection with experimental results, polymer physics represents a powerful tool in deciphering the chromosome arrangement and dynamics.

CPP 60.2 Thu 15:30 ZEU 260

Minimal surfaces on unconcatenated polymer rings in melt — •Jan Smrek[1] and Alexander Grosberg[2] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Center for Soft Matter Research and Department of Physics, New York University, New York, NY 10003, USA

In order to quantify the effect of mutual threading on conformations and dynamics of unconcatenated and unknotted rings in the melt we computationally examine their minimal surfaces. We found a linear scaling of the surface area with the ring length. Minimal surfaces allow for an unambiguous algorithmic definition of mutual threading between rings. Based on it, we found that although ring threading is very frequent, vast majority of cases correspond to very short loops. These findings explain why approximate theories which neglect threading in the description of static and dynamic properties of ring melts are so unexpectedly successful despite having no small parameter justification. We also examine threading dynamics, and identify the threading order parameter that reflects the slowdown of the ring diffusion.

CPP 60.3 Thu 15:45 ZEU 260

Density effects in entangled solutions of linear and ring polymers — •Negar Nahali and Angelo Rosa — SISSA - Scuola Internazionale Superiore di Studi Avanzati, Via Bonomea 265, 34136 Trieste, Italy

We present here recent [1] findings from molecular dynamics computer simulations regarding the statics and dynamics of linear and circular (ring) polymer chains in entangled solutions of different densities.

While we confirm that linear chain conformations obey Gaussian statistics at all densities, rings tend to crumple becoming more and more compact as the density increases. Conversely, contact frequencies between chain monomers are shown to depend on solution density for both chain topologies.

The relaxation of chains at equilibrium is also shown to depend on topology, with ring polymers relaxing faster than their linear counterparts. Finally, we discuss the local viscoelastic properties of the solutions by showing that the diffusion of dispersed colloid-like particles is markedly faster in the rings case [1,2].

[1] N. Nahali, A. Rosa, Journal of Physics: Condensed Matter 28, 065101 (2016)

[2] N. Nahali, A. Rosa, in preparation.

CPP 60.4 Thu 16:00 ZEU 260

Slow diffusion of ring polymer melts originated from interring threading — •Eunsang Lee[1,2] and YounJoon Jung[1] — [1]Department of Chemistry, Seoul National University, Seoul 08826, Korea — [2]Institut für Physik, Martin-Luther Universität Halle-Wittenberg, Halle 06120, Germany

Topological constraints of a ring, nonconcatation and unknotting, force the rings to be in a threading configuration, which is believed to be a main reason for abnormally slow diffusion observed in a melt phase. In this presentation, we provide results for the threading dynamics using molecular dynamics (MD) simulation based on a bead-spring model and Monte Carlo simulation on a kinetically constrained lattice gas model. Threading configuration between two molecules frequently observed in MD trajectories causes asymmetric dynamic state of two molecules and a set of such rules is implemented in the lattice model to describe the ring diffusion. Both models well describe long-time behavior of the ring diffusion strongly governed by a long-lasting molecular contact from threading configuration. An evidence for the glassy dynamics is also presented to support the ring melt belonging to a topological glass. From this work, we gain physical insights on the relation between molecular topology and its slows dynamics of ring polymer melts.

CPP 60.5 Thu 16:15 ZEU 260

Topological Interactions in Dilute Polymer Solutions – Disentanglement of Two Single Chains — •Diddo Diddens[1], Nam-Kyung Lee[2], Sergei Obukhov[3], Jörg Baschnagel[1], and Albert Johner[1] — [1]Institut Charles Sadron, Université de Strasbourg, CNRS UPR22, 23 Rue du Loess, 67034 Strasbourg Cedex 2, France — [2]Institute of Fundamental Physics, Department of Physics, Sejong University, Seoul 05006, Korea — [3]Department of Physics, University of Florida, P.O. Box 118440, Gainesville, Florida 32611-8440, United States

The non-crossing constraint of individual polymer chains is a well-known feature that explains several dynamical characteristics of dense polymer solutions or melts. However, the situation becomes less clear when dealing with an ensemble consisting of only a few long polymer chains that overlap, a scenario that is frequently encountered in *e.g.* biopolymer physics. To assess the impact of topological constraints in dilute polymer systems in a general manner, we devise a hypothetical experiment in which a long polymer chain is cleaved into two distinct halves that initially overlap, and study their subsequent disentanglement via Molecular Dynamics simulations [1]. We demonstrate that the non-crossing constraint significantly affects the separation dynam-

ics, and quantify the associated relaxation times in terms of the topological properties of the starting configuration from which the cleavage is initiated. Moreover, we rationalize our findings by analytical arguments.
[1] D. Diddens *et al.*, *ACS Macro Lett.*, **2016**, 5(6), 740-744

15 min break

Invited Talk CPP 60.6 Thu 16:45 ZEU 260
Knots as Stable Topological Order Parameter for Semiflexible Polymers — •Wolfhard Janke and Martin Marenz — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany

We investigate the influence of bending stiffness on the conformational phases of a semiflexible bead-stick homopolymer and present the pseudo-phase diagram for the complete range of semiflexibility, from flexible to stiff. By varying the internal bending stiffness, the model exhibits different pseudo phases like bent, hairpin or toroidal. In particular, we find thermodynamically stable phases characterized by knots of specific topologies. The transitions into these "knotted" phases from other ordered phases are quite unusual in that they display clear phase coexistence but almost no change in the mean total energy and hence no latent heat. It will be explained how we arrive at these intriguing results by computer simulations based on a combination of the replica-exchange Monte Carlo algorithm and the multicanonical method and discussed how one can understand these effects by basic statistical physics reasoning.

M. Marenz and W. Janke, *Knots as a Topological Order Parameter for Semiflexible Polymers*, Phys. Rev. Lett. **116**, 128301 (2016).

M. Marenz and W. Janke, *Stable Knots in the Phase Diagram of Semiflexible Polymers: A Topological Order Parameter?*, J. Phys.: Conf. Ser. **750**, 012006 (2016).

CPP 60.7 Thu 17:15 ZEU 260
An application of the Wang-Landau Monte Carlo method to the modeling of the themal and mechanical behavior of knotted polymer rings in solutions — •Franco- Ferrari[1] and Yani Zhao[2] — [1]CASA* and University of Szczecin, Szczecin, Poland — [2]Centre of New Technologies, University of Warsaw, Warsaw, Poland

The subject of this seminar are the properties and behavior in solutions of single knotted polymer rings. These polymers are defined on a simple cubic lattice. Their statistical properties are investigated by computing the expectation values of a few observables, namely the specific energy, the specific heat capacity and the gyration radius. In the case in which the chain is stretched by a tensile force directed along the z-axis, the average height of the point in which the force has been applied is measured too. The averages are computed exploiting a variant of the Wang-Landau Monte Carlo method. The algorithm has been suitably accelerated and parallelized in such a way that it is possible to sample a large number (from tens to hundreds of billions) of knot conformations. Several types of knots have been considered, including the trefoil, the figure-eight, the cinquefoil knots and many others. From the performed analysis it turns out that knotted polymer rings have a rich variety of different behaviors that can be used in order to tune the properties of polymer materials containing such knots. For instance, these polymers swell faster or slower when heated depending on the type of the knot and on the kind of interactions between the monomers. During the talk some interesting features of the stress relaxation of knotted polymer rings after the stretching force is removed will also be shown.

CPP 60.8 Thu 17:30 ZEU 260
Geometry and topology of periodic filamentous structures — •Myfanwy Evans — Mathematics Institute, TU Berlin, Berlin, Germany

High symmetry dense packings of trees and lines in the two-dimensional hyperbolic plane can be projected to triply-periodic minimal surfaces. The resulting three-dimensional structures are space-filling, symmetric and entangled structures composed of multiple networks or filaments, which challenge current characterisation techniques particularly from the perspective of entanglement. In this talk, I will discuss the construction and characterisation of these complex entangled structures alongside applications from star terpolymer self-assembly to skin swelling.

CPP 60.9 Thu 17:45 ZEU 260
Three-Dimensional Nets from Hyperbolic Tilings — •Benedikt Kolbe — Technische Universität Berlin

A main focus of modern crystallography is to explore the systematic enumeration and construction of nets in Euclidean space. The EPINET project attempts to enumerate crystalline frameworks that arise as structures derived from hyperbolic tilings. Since hyperbolic geometry represents the most prevalent class of geometry not only in nature as a model of the geometry of minimal surfaces, but also mathematically, the use of hyperbolic surfaces to construct possible structures in 3-space is very natural. Among many others, this recipe has also led to deep results in topology from Thurston and others and is also used in modern descriptions of conformal field theory.

We focus on the study of those networks that one encounters typically in the material sciences-periodic structures. Therefore, to classify the emerging structures we employ Delaney Dress combinatorial tiling theory.

We will explain some of the mathematics and intuition involved in a new approach to enumerating the 3-dimensional structures that arise through hyperbolic tilings and give some results on the knotted networks they represent. This work is aimed at generalizing Delaney-Dress tiling theory and to develop a complexity ordering of different tilings.

The most prominent triply periodic minimal surfaces are used to illustrate the approach and provide first examples. The goal of this project is to ultimately construct systematically and order by complexity all networks that arise by decorations of hyperbolic surfaces.

CPP 61: Charged Soft Matter, Ionic Liquids and Polyions II

Time: Thursday 15:00–17:00 Location: ZEU 114

CPP 61.1 Thu 15:00 ZEU 114
Impact of Momentum Conservation on the Ion Transport Mechanism in Ionic Liquids in and out of Equilibrium — •Diddo Diddens[1,2], Volker Lesch[1], Jens Smiatek[3], and Andreas Heuer[1,2] — [1]Helmholtz-Institut Münster (IEK-12), Ionics in Energy Storage, Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster, Germany — [2]Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster, Germany — [3]Institute for Computational Physics, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

Ionic liquids (ILs) are promising electrolyte materials for batteries or supercapacitors, as the enormous number of possible cation-anion combinations allows their fine tuning to match specific demands. We use Molecular Dynamics simulations to get deeper and more systematic insights into the ion transport mechanism in ILs. In particular, we study the correlated motion of the individual ionic species, and demonstrate that momentum conservation plays a crucial role for the overall transport properties, as it constrains the net motion of all ions. Furthermore, we apply strong electric fields to investigate nonlinear contributions to the conductivity.

CPP 61.2 Thu 15:15 ZEU 114
Molecular Dynamics and Charge Transport in Polymeric Ionic Liquids — •Falk Frenzel[1], Jiayin Yuan[2], Pia Borchert[3], Veronica Strehmel[3], and Friedrich Kremer[1] — [1]Universität Leipzig — [2]MPI Potsdam - Golm — [3]Hochschule Niederrhein Krefeld

After a remarkable evolution over the last 30 years, nowadays Ionic Liquids (ILs) play an essential role in a wide variety of application areas, as in chemical industry, medicine, and even space technology. However, their low viscosity often excludes them as macroscopic stable components, for instance, in battery electrolytes or gas separator membranes. In order to overcome this constraint (and to satisfy the processing industry) the outstanding features of neat ILs are combined with the well controllable macroscopic properties of polymers, which leads to a novel class of materials known as Polymeric Ionic Liquids (PILs). Although PILs have already demonstrated remarkable performance in electrochemical devices (as in dye-sensitized solar-cells, actuators, or field effect transistors), most fundamental properties are basically not yet understood. In the current study, the chemical structure of PILs is systematically varied and, on the other hand, the measurement techniques of Broadband Dielectric Spectroscopy (BDS), Transmission Electron Microscopy (TEM) as well as Differential Scanning (DSC) and AC-Chip Calorimetry are strategically employed. Hence, one is able to investigate the underlying charge transport mechanism(s), molecular dynamics, polarization effects, and mesoscopic structures in PILs in detail.

CPP 61.3 Thu 15:30 ZEU 114

Surface composition of a binary system "Ionic Liquid/Lithium Salt", investigated by photoelectron spectroscopy — •Fabian Ullmann[1], Anna Dimitrova[1], Marcel Himmerlich[1], Oliver Höfft[2], Frank Endres[2], and Stefan Krischok[1] — [1]Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, Germany — [2]Institut für Elektrochemie, Technische Universität Clausthal, Germany

Since a decade, the binary systems Ionic-Liquids (ILs)/lithium-salt are widely used media in electrochemistry. They were shown to be an important component in electrolytes for Li-ion batteries, and it is already demonstrated that a number of refractory metals are successfully deposited in ILs only in the presence of Li+. In order to control the electrochemical processes, an understanding of molecular and ionic interactions, which occur prior the electrochemical reduction, is required and the influence of side reactions of the electrolyte with the ambient atmosphere has to be known. To this end Photoelectron spectroscopy in ultra-high vacuum (UHV) is a powerful tool, being accessible to the very low vapor pressure of many ILs. In this study we use two ionic liquids with a common anionic part: [Py1,4][Tf2N] and [EMIm][Tf2N], in which Li[Tf2N] was dissolved in different quantities. The surface composition of these binary mixtures was studied both (i) for samples handled and transported to the UHV chamber solely under inert atmosphere and (ii) for those exposed to air before introducing them into the measurement system.

CPP 61.4 Thu 15:45 ZEU 114

Improving the Lithium Ion Transport in Polymer Electrolytes by Functionalized Ionic-Liquid Additives — Diddo Diddens[1,2], Volker Lesch[1], and •Andreas Heuer[1,2] — [1]Helmholtz-Institut Münster (IEK-12), Ionics in Energy Storage, Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster, Germany — [2]Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster, Germany

Polymer electrolytes consist of a salt dissolved in an amorphous polymer matrix, resulting in mechanically stable and flexible ion conductors. Unfortunately, their conductivity is too low for their use in modern energy storages. To overcome this deficiency, the addition of a low-molecular additive such as an ionic liquid (IL) has been proposed, however, the resulting enhancement is rather modest. Our recent work [1] demonstrated that this stems from the fact that the lithium ions remain coordinated to the slow polymer chains, which move only slightly faster due to the plasticization by the IL. To decouple the lithium ions from the macromolecular host, the use of a functionalized IL with chemically tethered oligomer chains that directly coordinate to the lithium ions has been suggested. We employ Molecular Dynamics simulations to investigate the lithium ion transport mechanism in these improved materials, and compare the results to conventional polymer electrolytes within the framework of our previously developed Rouse-based model [1].
[1] D. Diddens, A. Heuer, *ACS Macro Lett.*, **2013**, 2(4):322-326

CPP 61.5 Thu 16:00 ZEU 114

^{1}H and ^{7}Li NMR Diffusion and Relaxation measurements of PPG-LiClO$_4$ polymer electrolytes — •Simon Becker and Michael Vogel — Institut für Festkörperphysik, TU Darmstadt, Germany

Polymer electrolytes have been studied since the 1970s as applications for electrical devices because of low costs and mechanical flexibility. To understand effects of polymer-ion couplings on the charge transport in these materials, we use ^{1}H and ^{7}Li NMR. Moreover, we employ relaxometry and diffusometry methods to investigate dynamics on local and mesoscopic scales, respectively. We focus on mixtures of poly(propylene) glycol with lithium perchlorate in various concentrations. For these samples ^{1}H and ^{7}Li relaxation measurements revealed a strong slow down of segmental motion and ion dynamics with increasing salt concentration. In particular a linear relation between the position of the temperature-dependent ^{1}H T_1-minimum and the ion:monomer fraction was observed for the polymer backbone protons. The methyl group spin-lattice relaxation was unaffected by the salt content. The diffusion measurements showed a VFT behaviour of the polymer with reduced diffusivity and fragility for high salt concentrations.

CPP 61.6 Thu 16:15 ZEU 114

Conductivity Enhancement in Plastic Crystals — •Daniel Reuter, Korbinian Geirhos, Peter Lunkenheimer, and Alois Loidl — Experimental Physics V, University of Augsburg, Germany

Solid-state electrolytes for usage in lithium-ion batteries offer various advantages compared to their liquid counterparts. These are, e.g., design flexibility and higher safety [1]. Plastic crystals (PC) are promising candidates for such solid-state electrolytes. The molecules in a PC are ordered on a regular crystalline lattice while still exhibiting rotational motion. This rotational motion is believed to support ionic mobility in these materials. Interestingly, the ionic conductivity of the PC succinonitrile can be strongly enhanced by doping with ions [2] and admixing molecules [3]. This conductivity enhancement strongly depends on type of dopant and admixed molecule, which opens up a new research field on PCs. In this contribution, we provide dielectric and conductivity data for various mixed plastic-crystalline systems with ion addition.
[1] J. Motavalli, Nature **526**, 96 (2015). [2] P. Alarco *et al.*, Nature **3**, 476 (2004). [3] K. Geirhos *et al.*, J. Chem. Phys. **143**, 081101 (2015).

CPP 61.7 Thu 16:30 ZEU 114

Study of electrolyte structure and dynamics in Li-S batteries using molecular dyamics simulations with charge-scaling — •Chanbum Park[1,2] and Joachim Dzubiella[1,2] — [1]Helmholtz-Zentrum Berlin for materials and energy, 14109 Berlin, Germany — [2]Department of Physics, Humboldt-University of Berlin, 12489 Berlin, Germany

In the recent years, fundamental studies and the development of rechargeable batteries have been focused mostly on the design of cathode materials. Meanwhile, it has become clear that the role of electrolytes are important to improve the current batteries' performance. Molecular dynamics simulations are a good tool to investigate solubility, solvation and transport properties in batteries. Classical molecular dynamics simulations with non-polarizable force fields are able to produce physical properties and commonly used in physics and chemistry. Yet, the non-polarizable force fields simulations become problematic in low/non-polar solvents due to the fixed point charges. Leontyev et al, suggested molecular dynamics in electronic continuum (MDEC) to avoid this shortcoming of the non-polarizable force fields by scaling the ionic charges. In this study, molecular dynamics simulations with the MDEC approach to investigate the mixture of DME/DIOX with two lithium salts, lithium nitrate and lithium bistrifluoromethanesulfonamide (LiTFSI) are performed. Physical properties such as radial distribution function, coordination number, diffusion coefficient and conductivity are examined. In addition, the transport properties in pore structures and the effects of confinement are discussed.

CPP 61.8 Thu 16:45 ZEU 114

A lattice model to describe lithium ion batteries: insights from Monte Carlo simulations — •Alina Wettstein, Oliver Rubner, and Andreas Heuer — Institut für Physikalische Chemie, Corrensstraße 28-30, 48149 Münster, Deutschland

Numerous theoretical models have been developed in order to unravel the complex processes which occur in battery electrodes and electrolytes.

While some approaches account for molecular details by employing quantum chemical, molecular dynamics or continuum Monte Carlo calculations, other methods chose a macroscopic ansatz describing the battery cell as a whole system.

Here we present a lattice Monte Carlo (MC) model which seeks to bridge this gap of time and length scales by incorporating molecular and macroscopic parameters. Our MC model is designed as a modular system, which includes the internal electrochemical processes as well as the particle motion given the relevant interactions and rates within a cell. We study how to compute the major electrical properties of a battery, such as voltage and capacity, with a minimum input of outer parameters and test the influence of molecular properties, for example activation barriers, from MD simulations. With the help of this simplified, but highly flexible approach it is possible to further understand the basic principles of Li-batteries.

CPP 62: Fluids and Interfaces III

Time: Thursday 15:00–18:15 Location: ZEU 255

CPP 62.1 Thu 15:00 ZEU 255

Wedge wetting by an electrolyte solution — •Maximilian Mussotter and Markus Bier — Max Planck Institute Int. Sys. and University of Stuttgart, Germany

Wetting of substrates by fluids is a phenomenon of enormous importance in nature and technology. Whereas the highly idealised set-up of flat substrates in contact with simple fluids has been addressed intensively in the past, there is a huge practical interest in more realistic, and typically more complex, situations. A rather simple deviation from a flat substrate is a wedge-shaped wall, whose wetting properties by simple fluids have been studied for decades. An important phenomenon occurring in that context is the filling of a wedge, pre-empting the wetting transition of a planar wall.

Here, as a step towards more realistic set-ups, the wetting of a wedge by an electrolyte solution is considered, because many real fluids contain ions and electrostatic effects typically play a dominating role in the structure formation. One of the most remarkable findings of our study is the change of the order of the filling transition from a continuous transition for small surface charge densities to a first-order transition for large surface charge densities.

CPP 62.2 Thu 15:15 ZEU 255

Wetting over pre-existing liquid films - a tsunami on microscale — •Hannu Teisala, Anke Kaltbeitzel, Werner Steffen, Hans-Jürgen Butt, and Doris Vollmer — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Wetting of solids by liquids is a ubiquitous phenomenon of our everyday life. It is of utmost importance in several industrial operations including variety of coating applications, self-cleaning, oil recovery, heat transfer, and water harvesting from humid air. Static wetting situations, where the surface tension forces, γ, between solid, liquid, and gas phases balance with gravity leading to an energetically favored equilibrium state, are rather well understood. Comprehension of dynamic wetting situations, which are more common in real environment, is a challenge. Especially, wetting over pre-existing liquid films and the hydrodynamics within menisci - which are determined by the interplay of surface tension forces, gravity, and viscous stresses within the liquid - are poorly understood. Here we show how negative Laplace pressure acting at the meniscus of silicone oil, a common lubricant, induces a strong capillary suction that dominates the interface curvature and hydrodynamics when the meniscus is resting on or advancing over a thin film of the same liquid. The drastic consequences of negative Laplace pressure in wetting over liquid films have not been recognized earlier. Our findings add knowledge in the field of wetting and contribute to resolving generic issues such as homogeneous film formation in coating and meniscus formation, its hydrodynamics, and depletion of lubricant on slippery, lubricated surfaces.

CPP 62.3 Thu 15:30 ZEU 255

Comparing models of electrolyte solutions at curved electrodes — •Andreas Reindl, Markus Bier, and Siegfried Dietrich — Max Planck Institute for Intelligent Systems, Stuttgart, Germany

The proper functioning of many natural and artificial systems relies on an electrically charged substrate in contact with an electrolyte solution. As real substrates are typically rough, one has to reckon with properties deviating from those of idealised models based on smooth planar walls. In the present study we consider electrolyte solutions in contact with curved electrodes of spherical and cylindrical shape. Whereas these types of wall shapes have been investigated already in the past, the previous studies concentrated on specific models, without comparing different levels of sophistication. Here a variety of models within density functional theory are applied in order to describe the structure of the electrolyte solutions, and the differential capacitance was chosen as the central observable to characterise the electrical double layer. This procedure facilitates to compare results of different model calculations as a function of the electrode curvature. The mesoscopic Poisson-Boltzmann description allows for a detailed analysis and can be used as a gauge for more complex models. Within the so-called civilized model microscopic details such as particle volumes and solvent molecules with embedded dipole moments are taken into account. The influence of these microscopic parameters can be judged in comparison with simpler models.

Reference: A. Reindl, M. Bier, and S. Dietrich, in preparation.

CPP 62.4 Thu 15:45 ZEU 255

Influence of surfactants in forced dynamic dewetting — •Günter. K. Auernhammer, Franziska Henrich, Daniela Fell, Dorota Linke, and Hans-Jürgen Butt — MPI Polymer Research, Mainz, Germany

In this work we show that the forced dynamic dewetting of surfactant solutions depends sensitively on the surfactant concentration. Anionic, cationic and nonionic surfactants with critical micelle concentrations (CMCs) spanning four orders of magnitude were used. The receding contact angle in water decreased with increasing velocity. This decrease was strongly enhanced when adding surfactant, even at surfactant concentrations of 10% of the critical micelle concentration (1). Plots of the receding contact angle- versus-velocity almost superimpose when being plotted at the same relative concentration (concentration/ CMC). Thus the rescaled concentration is the dominating property for dynamic dewetting. The charge of the surfactants did not play a role, excluding electrostatic effects. The change in contact angle can be interpreted by local surface tension gradients, i.e. Marangoni stresses, close to the three-phase contact line. The decrease of dynamic contact angles with velocity follows two regimes. Despite the existence of Marangoni stresses close to the contact line, for a dewetting velocity above 1–10 mm s^{-1} the hydrodynamic theory is able to describe the experimental results for all surfactant concentrations. Flow profiles at different length scales support the hydrodynamic interpretation of the governing mechanism.

(1) F. Henrich, et al. Soft Matter **12** (2016): 7782 - 7791.

CPP 62.5 Thu 16:00 ZEU 255

Elasto-Capillary Interactions in the Absence of a Contact Line — Marco Rivetti[1], Thomas Salez[2], Maxence Arutkin[2], Chung-Yuen Hui[3], Elie Raphael[2], and •Oliver Bäumchen[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), D-37077 Göttingen, Germany — [2]UMR Gulliver, CNRS and ESPCI ParisTech, PSL University, Paris, France — [3]Department of Mechanical and Aerospace Engineering, Cornell University, Ithaca, NY, USA

A thin liquid film with non-zero curvature at its free surface spontaneously relaxes towards a flat configuration. This flow is driven by Laplace pressure gradients and resisted by the liquid's viscosity. In the last few years, we have studied the dynamics of this system experimentally, numerically and analytically (e.g. Rivetti et al., Soft Matter 11, 2015, McGraw et al., PRL 109, 2012). Inspired by recent progresses on the wetting behaviour and the dynamics of liquid droplets on soft substrates, we here consider the relaxation of a thin viscous film supported by an elastic foundation. We present experiments involving thin PS films on PDMS substrates, where the dynamics of the liquid-air interface is monitored by AFM. In this system, Laplace pressure gradients not only drive the flow, but they also induce elastic deformations on the substrate. These deformations affect the flow and the shape of the liquid-air interface itself, giving rise to an original example of an elasto-capillary interaction that is not mediated by the presence of a contact line. We also discuss a theoretical model and simulations that describe the coupled evolution of the substrate-liquid and the liquid-air interface.

CPP 62.6 Thu 16:15 ZEU 255

Wettability characteristics in fractionally wet porous media: a variation of the Cieplak-Robbins model — •Weiwei Li[1,2], Martin Brinkmann[1,2], Michael Jung[1,2], Stephan Herminghaus[2], and Ralf Seemann[1,2] — [1]Universität des Saarlandes, Saarbrücken, Germany — [2]Max Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany

An extended two-dimensional model based on the seminal work of Cieplak and Robbins is developed to study the role that wettability plays in slow immiscible fluid displacement. The porous media in this model consists of two-dimensional disks, and the emerging series of local interfacial instabilities is controlled by the Laplace pressure, that drives the quasi-static motion of liquid fronts. Unlike the original CR model, we respect the possibility of advancing or retracting interfaces during periodic changes of the Laplace pressure. This variation of CR model allows us to study capillary saturation characteristics in fractionally wet disk packs. Different statistical processes are applied to generate bidisperse disk packs with positional disorder. The simulations for a drainage-imbibition cycle reveal that there is a minimum hysteresis loop opening in fractionally wet packs. Several potential explanations are examined and discarded, favoring a simple explanation in terms of the distribution of entry pressures for non-cooperative pore filling events.

15 min break

CPP 62.7 Thu 16:45 ZEU 255

Structural disjoining pressures from DFT and the spreading of terraced drops — •Uwe Thiele[1], Adam P. Hughes[2], Hanyu Yin[2], David N. Sibley[2], and Andrew J. Archer[2] — [1]Institut für Theoretische Physik, Westfälische Wilhelms-Universität, Wilhelm-Klemm Str. 9, 48149 Münster — [2]Department of Mathematical Science, Loughborough University, Loughborough, LE11 3TU, UK

For a liquid film on a solid substrate, we determine the binding potential $g(h)$ that encodes the wetting behaviour. The method developed in [1] for the example of a simple discrete lattice-gas model, is used with continuum density functional theory (DFT) to calculate the binding potential for a Lennard-Jones fluid and other simple liquids. The DFT we use incorporates the influence of the layered packing of molecules at the surface. At low temperatures this can result in an oscillatory decay of $g(h)$, i.e., a structural disjoining pressure $\Pi = -\partial g/\partial h$ [2]. The obtained binding potentials are incorporated in a mesoscopic hydrodynamic model to study the spreading of (terraced) drops on both, an adsorption (or precursor) layer and completely dry substrates [3]. To achieve this, the thin film model is modified in such a way that for thicker films the standard mesoscopic hydrodynamic theory is realised, but for very thin layers a diffusion equation is recovered. [1] A.P. Hughes, U. Thiele, and A.J. Archer, J. Chem. Phys. 142, 074702 (2015). [2] A.P. Hughes, U. Thiele and A.J. Archer, preprint at http://arxiv.org/abs/1611.06957. [3] H. Yin, D.N. Sibley, U. Thiele and A.J. Archer, preprint at http://arxiv.org/abs/1611.00390.

CPP 62.8 Thu 17:00 ZEU 255

Effects of thermal fluctuations on an interface near a contact line — Daniele Belardinelli[1], Mauro Sbragaglia[1], •Markus Gross[2,3], and Bruno Andreotti[4] — [1]Department of Physics & INFN, University of Rome ”Tor Vergata”, Via della Ricerca Scientifica 1, 00133, Rome, Italy — [2]Max-Planck-Institut für Intelligente Systeme, Heisenbergstr. 3, 70569 Stuttgart, Germany — [3]IV. Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [4]Physique et Mecanique des Milieux Heterogenes, UMR 7636 ESPCI-CNRS, Universite Paris-Diderot, 10 rue Vauquelin, 75005, Paris, France

We analytically study a liquid interface contacting a solid wall in the presence of interfacial and contact point fluctuations. A path integral description based on a contact potential is developed which takes fully into account the impenetrability of the wall. We do not assume the presence of a precursor film in front of the effective contact point, but, instead, treat the fluctuations of the contact point explicitly. As a consequence of entropic repulsion, the average profile is curved and a characteristic length scale given by the interfacial roughness emerges. The effect of fluctuations are captured in terms of an effective disjoining pressure. We identify a transition from a partial to a pseudo-partial wetting state, the latter being characterized by a precursor film of constant thickness. In the partial wetting state, instead, we find that the average profile is exponentially decaying in front of the mean contact point. Reference: D. Belardinelli, M. Sbragaglia, M. Gross, B. Andreotti, Phys. Rev. E 94, 052803 (2016)

CPP 62.9 Thu 17:15 ZEU 255

Aubry Transition in 2D Colloidal Crystals — •Thorsten Brazda — 2. Physikalisches Institut, Universität Stuttgart Pfaffenwaldring 57, 70550 Stuttgart, Germany

According to Aubry et al., the static friction of a monolayer of interacting particles sliding across a crystalline surface can completely vanish in incommensurate systems leading to superlubricity [1]. For a given amplitude of the substrate potential, there exists a critical value of the particle interaction strength above which the monolayer elastically slides across the substrate even for an infinitesimally small driving force. Below that value, the chain becomes locked to the substrate which leads to a finite static friction force. In our experiments we investigate an extended 2D colloidal crystal which is driven across a (111) substrate, the latter created by a laser interference pattern. When the lattice constant of the colloidal crystal is incommensurate with the length scale of the underlying substrate potential, we observe the disappearance of static friction for non-zero substrate strengths. In agreement with recent numerical simulations [2], our results suggest, that this Aubry transition is of first order and that this dynamical phase transition is accompanied by characteristic structural changes in the monolayer.

1. M. Peyrard, J. Phys. Chem. C: Solid State Physics, 1983. 16(9): p. 1593.
2. D. Mandelli, Physical Review B, 2015. 92(13): p. 134306.

CPP 62.10 Thu 17:30 ZEU 255

Spontaneous electrification of fluoropolymer-water interfaces probed by electrowetting — Arun Banpurkar[1,2], Yogesh Sawane[1], Sandip Wadhai[1,2], Chandra Murade[2], Igor Siretanu[2], Dirk van den Ende[2], and •Frieder Mugele[2] — [1]Pune University, Pune, India — [2]Univ. of Twente, Enschede, The Netherlands

Fluoropolymers are widely used as coatings for their robustness, water-repellence, and chemical inertness. In contact with water, they assume a negative surface charge, which is commonly attributed to adsorbed hydroxyl ions. Here, we demonstrate that a small fraction of these ions permanently sticks to Teflon AF and Cytop surfaces upon prolonged exposure to water. Electrowetting measurements carried out after aging in water are used to quantify the density of trapped charge. Values up to -0.07 and -0.2mC/m^2 are found for Teflon AF and for Cytop, respectively, at elevated pH. A similar charge trapping process is also observed upon aging in various non-aqueous polar liquids and in humid air. A careful analysis highlights the complementary nature of electrowetting and streaming potential measurements in quantifying interfacial energy and charge density. We discuss possible mechanism of charge trapping and highlight the relevance of molecular scale processes for the long term stability and performance of fluoropolymer materials for applications in electrowetting and elsewhere.

CPP 62.11 Thu 17:45 ZEU 255

Mesoscopic simulations of electrokinetic phenomena: electrowetting dynamics. — •Nicolas Rivas[1], Stefan Frijters[2], Ignacio Pagonabarraga[3], and Jens Harting[1,2] — [1]Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IEK-11), Nürnberg, Germany — [2]Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands. — [3]Departament de Física Fonamental, Universitat de Barcelona, Barcelona, Spain

Electrokinetic effects play a crucial role in many natural and technological systems, from the biological to nano-fluidics. Numerical simulations of conducting fluids present a significant challenge mainly due to the variety of length-scales involved, and the presence of two long-range interactions: hydrodynamic and electrostatic. We show an electrohydrodynamic mesoscopic model, discuss its validity, and focus on the electrowetting effect, where a droplet changes its contact angle with a substrate when an electric field is applied. The hydrodynamics of two fluids is solved using the lattice-Boltzmann method. Ions present in the solvents are considered at the level of the Nernst-Planck equation, which is solved via a finite-volume, finite-difference discretization, following the link-flux method. We show that the simulation scheme is robust and remains valid in a wide range of parameters. Furthermore, the model is able to quantitatively capture the electrowetting effect, and allows to study in detail the mechanisms that lead to the saturation of the contact angle.

CPP 62.12 Thu 18:00 ZEU 255

Jumping drops on superhydrophobic surfaces: controlling energy transfer by timed electric actuation — Zhantao Wang, •Dirk van den Ende, Arjen Pit, Rudy Lagraauw, Daniel Wijnperle, and Frieder Mugele — Univ. of Twente, Enschede, The Netherlands

Aqueous sessile drops are launched from a superhydrophobic surface by electric actuation in an electrowetting configuration with voltage pulses of variable duration. We show that the jump height, i.e. the amount of energy that is transferred from surface energy to the translational degree of freedom, depends not only on the applied voltage but also in a periodic manner on the duration of the actuation pulse. The jump height for a pulse of optimized duration is almost twice as high as the one obtained upon suddenly turning off the voltage after equilibrating the drop under voltage. Representing the drop as a simple oscillator, we show that optimum pulse duration is related to the eigenfrequency of the drop. From a general perspective, our experiments illustrate a generic concept to manipulate drops on functionalized surfaces by tuning the duration of actuation stimuli to the intrinsic dynamics of the drops such that they can be positioned in a controlled manner in different non-equilibrium configurations.

CPP 63: Keynote Lecture IV

Time: Friday 9:30–10:00 Location: ZEU 222

Invited Talk CPP 63.1 Fri 9:30 ZEU 222

Stimuli-Responsive and Switchable Polymer Brushes: Theoretical Concepts and Computer Simulations — •Jens-Uwe Sommer — Leibniz-Institut für Polymerforschung Dresden, Hohe Strasse 6, 01069 Dresden — Technische Universität Dresden, Institut für Theoretische Physik, Zellescher Weg 17, 01069 Dresden

Polymers densely anchored onto surfaces display properties which combine liquid and solid state behavior. While such polymer brushes resist dissolution, friction and solvent flow they are able to change their properties over some range by changing the conformational statistics of the polymers collectively. This makes it possible to synthesize polymer surfaces which react on environmental stimuli in various ways and even suddenly switch their physico-chemical properties. In this talk I will discuss several aspects of how to influence the properties of polymer brushes by the environmental conditions using simple theoretical concepts and coarse-grained simulation studies. Starting from one-component neutral and charged brushes in simple solvents, I will show how various conformational transitions can be induced in two-component brushes. Another possibility to obtain switchable polymer surfaces is to consider multi-component solvents. In particular the case of co-nonsolvency seems to be a possible route to induce discontinuous phase transitions in polymer brushes via a small change of environmental variables. This presentation highlights the unique potential of polymer systems to display a variety of phase transitions even on finite scales.

CPP 64: Organic-Inorganic Hybride Interfaces (joint session CPP/DS/HL, organized by DS)

Time: Friday 9:30–11:45 Location: CHE 91

CPP 64.1 Fri 9:30 CHE 91

Hybrid organic-inorganic nano-structures studied by HR-PES and HR-TEM — •Olga Molodtsova[1,2], Sergey Babenkov[1], Irina Aristova[3], Andrei Hloskovsky[1], Denis Vyalikh[4], Dmitry Smirnov[5], Karina Schulte[6], and Victor Aristov[1,3,7] — [1]DESY, Hamburg, Germany — [2]ITMO, Saint Petersburg,Russia — [3]ISSP RAS, Chernogolovka, Russia — [4]TU Dresden, Germany — [5]BESSY, Berlin, Germany — [6]Max-lab, Lund, Sweden — [7]TU Bergakademie, Freiberg, Germany

Morphology and the electronic properties of hybrid organic-inorganic systems, composed of metallic nanoparticles which are self-organized in organic semiconductor thin film of phthalocyanines complexes were studied by transmission electron microscopy and photoelectron spectroscopy using synchrotron radiation.

CPP 64.2 Fri 9:45 CHE 91

STM and PES Investigations of Organic-TMD Heterointerfaces: Self-Assembly and Energy Level Alignment — •Thorsten Schultz[1], Yuli Huang[2,3], Zhibo Song[2,3], Zijing Ding[2], Lain-Jong Li[4], Dongzhi Chi[2], Patrick Amsalem[1], Andrew Wee[3], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Germany — [2]Agency for Science, Technology and Research, Singapore — [3]National University of Singapore — [4]King Abdullah University of Science and Technology, Saudi Arabia

The growing interest in two-dimensional transition metal dichalcogenide (TMD) materials brings additional opportunities for interfacing with organic molecules to fabricate flexible organic/inorganic devices. However, the complex interfacial properties at the organic-TMD heterointerfaces, including the growth behavior and energy level alignment (ELA) that determine the device performance, are still not well understood. Combining scanning tunneling microscopy/spectroscopy (STM/STS) with photoemission spectroscopy (PES), we are able to probe the self-assembly of fluorinated fullerene C60F48 on single-layer WSe2 deposited on a graphite substrate and its interfacial electronic properties. From our studies it is found that the interfacial dipole together with charge transfer play critical roles in determining the phase evolution of the C60F48 molecules adsorbed on the surface, as well as the ELA at the C60F48/WSe2/graphite heterointerface.

CPP 64.3 Fri 10:00 CHE 91

Energy Level Control at ZnO/Organic Semiconductor Interfaces — •Raphael Schlesinger[1], Sylke Blumstengel[1], Stefanie Winkler[2], Johannes Frisch[1], Jens Niederhausen[1], Ruslan Ovsyannikov[2], Antje Vollmer[2], Fritz Henneberger[1], and Norbert Koch[1,2] — [1]Humboldt-Universität zu Berlin, Institut für Physik — [2]Helmholtz-Zentrum Berlin - BESSY II

Hybrid inorganic organic systems (HIOS) are promising candidates for future (opto-)electronic devices by taking advantage of the complementary beneficial properties of two different material classes. However, inadequate interfacial energy level alignment is an intrinsic obstacle to superior device function. Hence, to design efficient HIOS devices, understanding and controlling HIOS energy level alignment is a key factor.

In this contribution we employ molecular electron donor or acceptor interlayers to tune the work function (ϕ) of ZnO between 2.2 eV (by using the organometallic donor [RuCp*mes]$_2$) and 6.4 eV (by using F4TCNQ). Only for molecular acceptor adsorption, significant adsorption induced upward band bending of up to 0.9 eV is found within ZnO. Exploiting the huge ϕ modifications of ZnO, up- and downward HIOS energy level readjustments are shown, which realize ultimately low electron- or hole-injection barriers. Moreover, by using an OSC whose gap matches that of ZnO, the energy level offsets at the HIOS interface could be eliminated. This enables highly efficient, non-quenched energy transfer across the HIOS interface, which is usually inhibited by unfavorable energy level alignment.

CPP 64.4 Fri 10:15 CHE 91

Structure of van der Waals bound Hybrids of Organic Semiconductors and Transition Metal Dichalcogenides: the Case of Acene Films on MoS2 — •Tobias Breuer, Tobias Massmeyer, Alexander Mänz, Steffen Zoerb, Bernd Harbrecht, and Gregor Witte — Philipps-Universität Marburg, Germany

Transition metal dichalcogenides (TMDC) are important representatives in the emerging field of two-dimensional materials. At present, their combination with molecular films is discussed as it enables the realization of van der Waals bound organic/inorganic hybrids which are of interest in future device architectures. Here, we discuss the potential use of molybdenum disulfide (MoS_2) as supporting substrate for the growth of well-defined, crystalline organic adlayers. By this means, hybrid systems between the TMDC surface and organic compounds can be prepared, allowing for the profound investigation of mutual optical and electronic coupling mechanisms. As model system, we choose pentacene and perfluoropentacene as prototypical organic semiconductors and analyze their film formation on MoS_2(001) surfaces. In both cases, we observe smooth, crystalline film growth in lying molecular configuration, hence enabling the preparation of welldefined hybrid systems. By contrast, on defective MoS_2 surfaces both materials adopt an upright molecular orientation and exhibit distinctly different film morphologies. This emphasizes the importance of highly ordered TMDC surfaces with low defect density for the fabrication of well-defined hybrid systems.

[1] T. Breuer et al., PSS RRL (2016), DOI: 10.1002/pssr.201600320

15 min. break.

CPP 64.5 Fri 10:45 CHE 91

Real-Time Investigation during Au sputter deposition on polymer and SiOx surfaces. — •Matthias Schwartzkopf[1], André Rothkirch[1], Björn Beyersdorff[1], Calvin Brett[1], Marc Gensch[1], Wiebke Ohm[1], Oleksandr Polonskyi[2], Alexander Hinz[2], Thomas Strunskus[2], Adrian Haussmann[3], Franziska Löhrer[3], Volker Körstgens[3], Franz Faupel[2], Peter Müller-Buschbaum[3], and Stephan Roth[1,4] — [1]DESY, Notkestr. 85, D-22607 Hamburg — [2]CAU zu Kiel, Kaiserstr.2, D-24143 Kiel — [3]TUM, James-Franck-Str. 1, D-85748 Garching — [4]KTH, Teknikringen 56-58,SE-100 44 Stockholm

The reproducible low-cost fabrication of functional polymer-metal-nanocomposites remains a major issue in applied nanotechnology. In order to obtain full control over the nanostructural evolution at the metal-polymer interface, we employed the combination of time-resolved surface sensitive X-ray scattering with optical measurements during sputter deposition of gold on thin polystyrene films [1] and SiOx [2]. We correlate the evolution of the metallic layer morphology with changes in the key scattering features. This enabled us to identify the impact of substrate effects on the growth regimes with their specific thresholds and their resulting optical properties. Our study opens up the opportunity to improve nanofabrication of tailored metal-polymer nanostructures for organic electronics like photovoltaic applications and plasmonic-based technologies. [1] Schwartzkopf et al., ACS Appl. Mater. Interfaces 7, 13547 (2015); [2] Schwartzkopf et al., Nanoscale 5, 5053 (2013).

CPP 64.6 Fri 11:00 CHE 91

Analytical Study of Solution-Processed Nickel Oxide and its Application in Organic Electronics - (1) Photoelectron Spectroscopy — •Florian Ullrich[1,4], Valentina Rohnacher[2,4], Jakob Bombsch[3,4], Wolfram Jaegermann[1,4], and Eric Mankel[1,4] — [1]TU Darmstadt, Materials Science Institute — [2]University of Heidelberg — [3]TU Braunschweig — [4]InnovationLab

For the fabrication of efficient organic solar cells (OPV) suitable extraction layers are needed. A material fulfilling the requirements and leading to superior efficiencies in comparison to the standard material PEDOT:PSS is nickel oxide (NiO).

In this work we want to contribute to a more detailed understanding of the relations between annealing temperature of solution-processed NiO (sNiO), surface treatments, bulk and surface composition, structure and properties, ability to form self-assembled monolayers (SAMs) and the characteristics of sNiO-based OPV. For that purpose different analytical methods like x-ray photoelectron spectroscopy (XPS) and infrared spectroscopy (IR) were conducted and various OPVs were built and characterized.

In this first part we use XPS to monitor changes of band bending and surface dipoles induced by surface treatments like oxygen plasma (OP) or deposition of SAMs. These information help to explain characteristics of corresponding OPVs and provide valuable hints for the design of more efficient devices. We show how band alignment can controllably be improved by adjusting the work function via varying annealing temperature of sNiO films, OP treatment and SAM molecules.

CPP 64.7 Fri 11:15 CHE 91

Analytical study of Solution-processed Nickel Oxide and its Application in Organic Electronics: (2) Infrared Spectroscopy — •Valentina Rohnacher[1,2], Sabina Hillebrandt[1,2], Florian Ullrich[2,3], Jakob Bombsch[2,4], Sebastian Beck[1,2], and Annemarie Pucci[1,2] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg — [2]InnovationLab, Heidelberg — [3]TU Darmstadt — [4]TU Braunschweig

The performance of organic photovoltaic cells (OPVs) is significantly influenced by the properties of the interfaces between the layers. Increasing the interfacial compatibility especially between the transparent conductive oxide electrode and the organic semiconductor layer can improve the charge carrier transport through the stack and thus the efficiency of the device. Thin films of nickel oxide (NiO) have shown promising characteristics as hole extraction layers in OPVs. In our studies, solution-processed NiO surfaces were passivated by self-assembled monolayers (SAMs) to tune the work function and to reduce the surface reactivity. Infrared spectroscopy gives insight into the composition of the investigated material and can monitor orientation of characteristic vibrations or functional groups. The results show that temperature and plasma treatment dramatically change the surface properties and that especially nickel hydroxide and nickel oxyhydroxide play an important role for the binding mechanism of SAMs. Together with photoelectron spectroscopy and OPV device characteristics a better understanding of the energetic and chemical properties at the interface was achieved helping to improve device performance.

CPP 64.8 Fri 11:30 CHE 91

Analytical Study of Solution-Processed Nickel Oxide and its Application in Organic Electronics: (3) Application in Organic Solar Cells — •Jakob Bombsch[1,2,4], Sebastian Hietzschold[1,2,4], Valentina Rohnacher[2,4], Florian Ullrich[3,4], Robert Lovrincic[1,4], and Wolfgang Kowalsky[1,2,4] — [1]TU Braunschweig — [2]Uni Heidelberg — [3]TU Darmstadt — [4]InnovationLab, Heidelberg

Nickel oxide (NiO) has shown promising properties as a carrier-selective hole contact material with high transparency, and a good matching ionization potential to most donor materials [1,2]. Here we apply solution-processed NiO films as an interlayer in small molecule flat- and bulk-heterojunction solar cells with F4ZnPc and C60 as a donor and acceptor, respectively, and correlate the observed IV-characteristics with annealing temperature, thickness, and surface post-treatment of the NiO layer. While oxygen plasma treatment improves device performance, the application of dipolar self-assembled monolayers lead to strongly S-shaped IV curves. To examine the nature of the barrier introduced, we vary the doping density of the NiO film by adding copper oxide. Together with data from Infrared spectroscopy and Photoelectron spectroscopy measurements, we gain a more fundamental understanding of the impact of NiO surface properties on solar cell performance. [1] Manders, J. R. Et al. Adv. Funct. Mater., 23: 2993-3001 (2013). [2] Schulz, P. et al. Adv. Funct. Mater. 24, 701-706 (2014).

CPP 65: Complex Fluids and Soft Matter (organized by DY)

Time: Friday 9:30–12:30 Location: HÜL 186

Invited Talk CPP 65.1 Fri 9:30 HÜL 186

Liquid Crystals in Microgravity — •Ralf Stannarius — Otto-von-Guericke-Universität Magdeburg

Experiments under microgravity allow to study dynamic processes in thin freely suspended liquid films in air, as well as freely floating bubbles of smectic liquid crystals. These are representative for quasi-twodimensional liquids. Shape dynamics, film rupture, and mobility and interactions of inclusions in quasi-2D emulsions are topics of scientific interest in these unique fluid structures. Results from parabolic flights, a suborbital rocket flight, and an ISS experiment are presented.

CPP 65.2 Fri 10:00 HÜL 186

Temporal evolution of free floating smectic bubbles — •Patricia Dähmlow, Torsten Trittel, Christoph Klopp, Kirsten Harth, and Ralf Stannarius — Otto-von-Guericke University Magdeburg, Germany

Freely floating smectic bubbles are investigated under microgravity conditions, which form a minimal surface, like soap bubbles, in equilibrium. A great advantage of freely floating bubbles is the absence of a meniscus, which acts as a reservoir of smectic material when the surface area of the film changes. In this work, the freely floating bubble must rearrange its internal layer structure without such a reservoir. Bubbles are produced by collapsing catenoids, resulting in an elongated shape after the rupture of the catenoids. With time the bubble shows complex oscillations, which includes the invagination of the film and thus, a temporary increase of the surface area until it relaxes to a sphere. Experiments are performed performed with optical highspeed imaging during parabolic flights.

CPP 65.3 Fri 10:15 HÜL 186

Orientational order on surfaces - the coupling of topology, ge-

ometry and dynamics — •Axel Voigt, Michael Nestler, Ingo Nitschke, and Simon Praetorius — Institut für Wissenschaftliches Rechnen, TU Dresden, Germany

We consider the numerical investigation of surface bound orientational order using unit tangential vector fields by means of a gradient-flow equation of a weak surface Frank-Oseen energy. The energy is composed of intrinsic and extrinsic contributions, as well as a penalization term to enforce the unity of the vector field. Four different numerical discretizations, namely a discrete exterior calculus approach, a method based on vector spherical harmonics, a surface finite-element method, and an approach utilizing an implicit surface description, the diffuse interface method, are described and compared with each other for surfaces with Euler characteristic 2. We demonstrate the influence of geometric properties on realizations of the Poincare-Hopf theorem and show examples where the energy is decreased by introducing additional orientational defects.

CPP 65.4 Fri 10:30 HÜL 186

Microrheology of rod-shaped particles in free standing liquid crystal films of the smectic phase — •Christoph Klopp, Alexey Eremin, and Ralf Stannarius — Institute of Experimental Physics, Otto-von-Guericke University Magdeburg, Germany

Flow phenomena in restricted geometries have been studied in a variety of different physical, chemical and biological systems in the last years. These studies investigate the motion of proteins in lipid membranes and the motion of submicrometer-sized inclusions on thin membranes. Organic liquid crystal materials are able to form very thin, stable free standing films of highly uniform structure and thickness, making them ideal systems for studies of hydrodynamics in two dimensions. We study the mobility of sphere and rod-shaped inclusions in freely-suspended liquid crystal films of the smectic A phase [1]. For the rod-shaped particles we analyze the rotational and translational mobility by measuring Brownian motion. We compare our results with the existing theory of Saffman and Delbrück [2] and analyze the effect of particle anisometry. Measurable effects appear when the length of the particles is comparable to or larger than the hydrodynamic size of the system (Saffman length) and we are able to confirm the theory of Levine et al. with our data [3].

[1] A. Eremin *et al.*, 2011. Pys. Rev. Lett. 107, 268301.
[2] Z. H. Nguyen *et al.*, 2010. Pys. Rev. Lett. 105, 268304.
[3] A. J. Levine *et al.*, 2004. Phys. Rev. Lett. 93, 038102.

CPP 65.5 Fri 10:45 HÜL 186

Structure and rheology of suspensions controlled by capillary forces in thin liquid films — •Andrea Scagliarini[1] and Jens Harting[1,2] — [1]Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IEK-11), Nürnberg, Germany — [2]Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands

Commonly, the rheology of suspensions is primarily controlled by the volume fraction of solids, as it is the case, for instance, of colloidal gels. However, it has been recently shown that adding small amounts of a liquid, immiscible with the continuous phase of the suspension, affects strikingly the mechanical response of the system, even at low solid volume fraction, owing to the formation of particle aggregates and networks sustained by capillary forces. Such structures endow the material with elasto-plastic/gel-like properties which make these capillary suspensions particularly suitable for a number of applications. By means of lattice Boltzmann simulations I will address a number of open questions, concerning: i) the dependence of the network structure upon the particle shape and wettability, and, in turn, ii) the dependence of the rheological properties on such structure. In particular, I will show that by adding water to an oil-based suspension of strongly hydrophobic particles, the formation of a percolating cluster is observed. The percolation transition occurs at a critical value of the water volume fraction, for which we provide an explicit expression depending of the particle geometry, the solid volume fraction and the contact angle.

CPP 65.6 Fri 11:00 HÜL 186

Transient dynamics in the accelerating region of collapsing freely suspended films — •Florian von Rüling and Alexey Eremin — Institute of Experimental Physics, Otto von Guericke University Magdeburg, Universitätsplatz 2, 39016 Magdeburg, Germany

We report experimental studies on collapse dynamics of freely suspended smectic liquid crystal films. In contrast to soap films, whose collapse has been studied in detail, films of thermotropic liquid crystals have a well-defined layer structure and represent a quasi-two-dimensional fluid. The particular inner structure of smectics stabilizes freely suspended films with an extraordinary surface-to-volume-ratio. In our studies, we use tracer particles to visualise the flow in collapsing smectic films, thus enabling us to estimate the size of the dissipation region and to test the predictions of the theory. Using high-speed imaging we show that the advective flow involves the whole film, however, the flow velocity gradually reduces with the distance from the moving edge. The dissipation region is nearly independent of the film thickness.

15 min. break

CPP 65.7 Fri 11:30 HÜL 186

A nearly incompressible mesoscopic method for simulating complex fluids and flows — •Davod Alizadehrad and Dmitry A. Fedosov — Institute of Complex Systems and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

Numerical simulation and theoretical modeling of mesoscopic processes are constantly challenged by the large separation of time scales and length scales. We introduce a general mesoscopic framework for simulating complex liquids and flows using the smoothed dissipative particle dynamics [1]. Modifying the equation of state and the course-grained system, we show that the speed of sound can be controlled, while the radial distribution function (RDF), the mean-square displacement, and the Schmidt number correspond to liquid state, even for low temperatures. Performing reverse-Poiseuille flow simulations, measured viscosity shows only 1-2 percent changes over several orders variation of shear rates. The RDF in equilibrium and in shear flow remains same and independent of shear rates. This is an advantage in modeling of structures and boundaries either rigid or deformable. As a challenging test of incompressibility, we have considered the Poisson ratio, divergence of velocity field, and the number density in elongational flow. Density variation remains smaller than one percent and the velocity field satisfies well the divergence-free condition, indicating that the simulated fluid is nearly incompressible. Finally, we present the applicability and validity of the method in simulating cellular blood flow in irregular geometries as an example of complex mesoscopic fluids flow.

[1] K. Müller, et al., J. Comp. Phys. **281**, 301-315, (2015)

CPP 65.8 Fri 11:45 HÜL 186

How to regulate the position of a droplet in a heterogeneous liquid environment? — •Samuel Krüger[1,2], Christoph A. Weber[4], Jens-Uwe Sommer[2,3], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Leibniz Institute of Polymer Research Dresden e.V. — [3]Technische Universität Dresden, Institute of Theoretical Physics, Dresden, Germany — [4]Harvard University, Division of Engineering and Applied Sciences, Cambridge, USA

Cells contain organelles that are not separated from the cytoplasm by a membrane. An example are liquid-like P granules in the *C. elegans* embryo. P Granules consist of RNA and proteins that are segregated from the cytoplasm. During asymmetric cell division, P granules are segregated to one side of the cell and distributed to only one daughter cell. This segregation is guided by the spatial concentration gradient of the protein Mex-5. Motivated by this system, we study the general question of how droplets are positioned in a concentration gradient of a regulator molecule that influences phase separation. We consider a ternary system and study the simplified case, where an external potential establishes the regulator gradient. A mean field Flory-Huggins model reveals a first order phase transition between the droplet position at high and low regulator concentration. We discuss this result in comparison to Monte Carlo simulations. Simulations reveal signatures of the mean field phase transition and give insight into the free energy landscape of the system in the presence of fluctuations.

CPP 65.9 Fri 12:00 HÜL 186

Self-Assembly of Rings and Capsids in Hydrodynamic Flow — •Nikolas Schnellbächer[1,2], Fabian Fuchs[1,2], and Ulrich Schwarz[1,2] — [1]Institute for Theoretical Physics, Heidelberg University, Germany — [2]BioQuant, Heidelberg University, Germany

Patchy particle systems have emerged as useful model systems to investigate protein or colloidal self-assembly, but are usually studied under ideal conditions. We study self-assembly of patchy particles in hydrodynamic flow since this is a typical scenario for many applications and represents an important step towards more complex environments. Solute particles are propagated using Molecular Dynamics (MD) with solute-solute reactions being implemented through reactive patches. Solvent flow is simulated with Multi-Particle Collision Dynamics (MPCD). As paradigmatic examples, we study the assembly of pentagonal rings and icosahedral capsids with and without hydrodynamic flow. We find that there is a strong nonlinear relationship between shear rate and assembly yield and observe a multi-pitched interplay between shear rate and frequency of malformed complexes. This leads to optimal regimes both at low and intermediate shear rates, such that a balanced relation of bond association and dissociation prevents kinetic trapping and ensures constant monomer supply. At very high shear assemblies are disrupted by force. Our work highlights how both strong cooperative effects and non-equilibrium conditions are important to understand the intricate dynamics of self-assembly pathways.

CPP 65.10 Fri 12:15 HÜL 186

Regulation of liquid phase separation of PGL-3 protein by RNA — •Omar Adame-Arana[1], Christoph A. Weber[1,2], Shambaditya Saha[3], Anthony A. Hyman[3], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [2]Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA — [3]Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden, Germany

Liquid-liquid phase separation has been proposed as a key mechanism for the assembly and maintenance of membraneless compartments in cells. For example, in the *C. elegans* embryo, liquid-like droplets called P granules, condense and subsequently segregate to one side of the cell prior to cell division. P granules play a key role in the specification of germ cell fate. It has been shown that PGL-3, a key P granule component, is able to form RNA-rich liquid droplets in vitro. We investigate the role of RNA to facilitate phase separation using a Flory-Huggins model. We show that competition for RNA binding by PGL-3 and the regulatory protein Mex-5 can acount for the observed droplet segregation.

CPP 66: Glasses and Glass Transition (joint session DY/CPP/DF, organized by DY)

Time: Friday 10:00–12:30 Location: ZEU 118

CPP 66.1 Fri 10:00 ZEU 118

Molecular Dynamics Simulations of Aqueous Mixtures in Bulk and Nano-Confinement — •Niels Müller, Rebecca Schmitz, and Michael Vogel — Institut für Festkörperphysik, Technische Universität Darmstadt

Binary mixtures of glass forming liquids have complex dynamical properties, leading to shifted time scales of the dynamics or changed temperature dependence compared to the respective behavior of the pure liquids. We performed MD simulations of ethylene-glycol water mixtures in silica-pores, which show unmixing near the pore wall and a change from non-Arrhenius to Arrhenius like temperature dependence. To single out the origin of these unusual behaviors we use binary mixtures composed of two water-like molecules with different polarity as a model system. These systems avoid steric effects from molecules of different size and have the characteristic tetrahedral order of water, but form hydrogen bonds of different strength. Through simulations in a wide temperature range we probe unmixing transitions of these systems. In addition, we confine these model mixtures by walls formed by fixed molecules of one of the water-like species. In this way, we systematically study the effect of the polarity of the confinement on mixtures of hydrogen-bonded liquids. Performing spatially resolved analyses or selecting a subset of the system we can gather detailed insights into the effects of confinement on the dynamics of these systems.

CPP 66.2 Fri 10:15 ZEU 118

The glass transition as a mixture of random organization and athermal jamming — Moumita Maiti and •Michael Schmiedeberg — Institut für Theoretische Physik 1, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

We explore the properties of the glass transition by employing a model system for a mixture of athermal jamming and random organization. We start with random configurations of soft repulsive spheres. While athermal jamming is realized by heading for the local minimum of the overlap energy without crossing energy barriers, random organization is obtained if we displace overlapping particles randomly in each step [1]. When mixing these protocols, we obtain a transition which is in the universality class of a directed percolation transition in time. Furthermore, we reveal that the limit of a small but nonzero probability of random steps differs from the case without random steps. This limit corresponds to the glass transition at small but non-zero temperatures. As a consequence the glass transition is a directed percolation transition and is fundamentally different from the athermal jamming transition. Finally, we explore the relation to spatial percolation transitions.

[1] L. Milz and M. Schmiedeberg, Connecting the random organization transition and jamming within a unifying model system, Phys. Rev. E 88, 062308 (2013).

CPP 66.3 Fri 10:30 ZEU 118

NMR and BDS Experiments on Water confined in MCM-41 — •Edda Klotz, Matthias Sattig, Christina Lederle, and Michael Vogel — TU Darmstadt Solid State Physics, Darmstadt, Germany

The investigation of the dynamics of water in confinement is relevant for various fields of interest, from biological applications to geological ones. It is well established that confined water undergoes a dynamic crossover upon supercooling. However, the origin of the crossover is controversially discussed. To further study this issue, we focus on water im MCM-41 silica nanopores and use por diameters for which well defined partial freezing occurs. Calorimetric studies are performed to characterize this freezing behavior. Moreover, nuclear magnetic resonance (NMR) and broadband dielectric spectroscopy (BDS) are applied to ascertain the dynamics of the non-freezing water fraction cross the freezing transition. The dielectric spectra exhibit several processes that are sensitive to an appearance of a solid water fraction. ^{2}H-NMR allows us to show that one of the processes can be identified with the rotational motion of water, exhibiting a kink in the temperature depenence at the freezing-transition. Moreover, ^{1}H static field gradient NMR yields self-diffusion coefficients of water, which can be linked to freezing-affected polarization processes in BDS. Thus, these combined studies clearly show a dynamic crossover due to formation of a solid water fraction.

CPP 66.4 Fri 10:45 ZEU 118

Water Dynamics in Mesoporous Silica Confinement — •Max Schäfer, Edda Klotz, Alexander Hariri, and Michael Vogel — Institut für Festkörperphysik, TU-Darmstadt, Germany

Confinement effects on the dynamics of water are examined using mesoporous silica MCM-41 with various pore diameters. Additionally the size of these pores are systematically modified by atomic layer deposition with Al2O3. To explore rotational motion, we combine different 2H NMR technics that are sensitive to molecular reorientations. Applying spin-lattice-relaxation, line shape analyzes and stimulated echo experiments, we cover the dynamical range down to very slow dynamics in a deeply supercooled temperature regime. 1H diffusion measurements in an ultra high static field gradient were performed also. These experiments were supplemented by broadband dielectric spectroscopy and differential scanning calorimetry. We find that the temperature dependence of the structural alpha-relaxation exhibits a kink, which is strongly related to the pore size. We show that this kink is not associated to a proposed liquid-liquid phase transition of water, but to partial freezing. Furthermore we study confinement effects on dynamics and phase behavior in binary mixtures of water and glycerol for various concentrations. The properties of the hydrogen bond network and an eventually phase separation initiated by the confinement are of great interest. Glycerol dynamics for confined mixtures show an Arrhenius behavior at low temperatures in contrast to bulk mixtures and to pure glycerol confined in MCM-41. The similarity to water dynamics in confinement suggests a cooperative motion of water and glycerol.

CPP 66.5 Fri 11:00 ZEU 118

Dynamical coexistence in a polydisperse hard-sphere liquid — •Matteo Campo[1,2], Christopher Patrick Royall[3], and Thomas Speck[1] — [1]Institut für Physik, Johannes Gutenberg-Universität, Mainz, Germany — [2]Graduate School Materials Science in Mainz, Germany — [3]H.H. Wills Physics Laboratory, University of Bristol, United Kingdom

The glass transition is a long-standing challenge of condensed matter physics. One of the problems is that no significant change in the global structure seems to arise upon vitrification [1]. Recent studies however have recovered the old idea of Frank according to which geometric motifs which minimise the local free energy, so-called locally favoured structures (LFS), would grow in correlation with the slow regions of the glass and thus play an important role in the transition [2]. Among the key insights is the identification of a non-equilibrium phase transition in trajectory space, which implies phase coexistence between a slow phase rich in LFS and the normal supercooled liquid. Here we present a study of a polydisperse hard-sphere model glassformer and its LFS properties upon crystallization [3] and vitrification. We combine our numerical simulations with experimental observations that support the picture of the non-equilibrium phase transition in trajectory space.

[1] Ludovic Berthier and Giulio Biroli. REV MOD PHYS, 2011.

[2] C Patrick Royall and Stephen R Williams. PHYS REP, 2015.

[3] Matteo Campo and Thomas Speck. JSTAT, 2016.

15 min. break

CPP 66.6 Fri 11:30 ZEU 118

Electro-diffusion versus chemical diffusion in alkali calcium phosphate glasses - implication of structural changes — •Anneli Hein, Johannes Martin, Martin Schäfer, and Karl-Michael Weitzel — Philipps-Universität Marburg

A long term transport experiment has been performed on a bioactive calcium phosphate glass of the molar composition 30 CaO *25 NaO *45 P2O5 using the technique of bombardment induced ion transport (BIIT) with potassium as foreign bombarder ion. Ion transport due to gradients of the electrical potential and the concentration lead to incorporation of K+ and depletion of both Na+ and Ca++ by electro-diffusion in forward direction. The resulting concentration profile has been quantitatively analyzed by ToF-SIMS. Further analysis of the P+ and POx+ signals (x = 1-4) shows characteristic changes of the structure of the local glass network. Since the concentration profiles imprinted by the BIIT constitute pronounced concentration gradients, these depletion profiles further evolve on a much longer time scale due to chemical diffusion (absence of electric potential gradients). The former depletion zone is partially refilled by chemical diffusion. At the same time the structural changes of the glass network are demonstrated to be reversible. Numerical simulations on the basis of the coupled Nernst-Planck-Poisson equations allow deriving the diffusion coefficients of sodium, potassium and calcium for both cases, i.e. electro-diffusion and chemical diffusion. The two experiments are sensitive to different aspects of the diffusion coefficients and thus are complementary.

CPP 66.7 Fri 11:45 ZEU 118

Confinement effects on the correlation of plasticity in amorphous solids — •Muhammad Hassani, Philipp Engels, and Fathollah Varnik — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr Universität, Bochum, Germany

In amorphous solids, spatio-temporal correlations of plastic deformation are known to be mediated by the elastic medium [1]. Solid walls may strongly alter this elastic propagator and are thus expected to also influence these correlations. We study this issue via large scale molecular dynamics (MD) simulations. Spatial correlations of plastic activity are found to decay more slowly when approaching a wall. This observation is paralleled by a similar trend in the case of the strain field around a spherical inclusion placed at various distances from a wall. Results obtained from MD simulations are in quantitative agreement with numerical solution of continuum mechanics equations in the presence of an inclusion [2,3].

[1] F. Varnik, S. Mandal, V. Chikkadi, D. Denisov, P. Olsson, D. Vagberg, D. Raabe, and P. Schall, Correlations of plasticity in sheared glasses, Phys. Rev. E 89, 040301 (2014)

[2] A. Nicolas and J.-L. Barrat, A mesoscopic model for the rheology of soft amorphous solids, with application to microchannel flows, Faraday Discuss. 167, 567 (2013)

[3] M. Hassani, P. Engels, and F. Varnik, Confinement effects on the correlation of plasticity in amorphous solids (in preparation

CPP 66.8 Fri 12:00 ZEU 118

Glass transitions, semiconductor-metal (SC-M) transitions and fragilities in Ge-V-Te (V=As, or Sb) liquid alloys: the difference one element can make — •Shuai Wei[1], Garrett Coleman[2], Pierre Lucas[2], and C.Austen Angell[1] — [1]Arizona State University — [2]University of Arizona

Glass transition temperatures (Tg) and liquid fragilities are measured along a line of constant Ge content in the system Ge-As-Te, and contrasted with the lack of glass-forming ability in the twin system Ge-Sb-Te at the same Ge content. The one composition established as free of crystal contamination in the latter system shows a behavior opposite to that of more covalent system. Comparison of Tg vs bond density in the three systems Ge-As-chalcogen differing in chalcogen i.e. S, Se, or Te, shows that as the chalcogen becomes more metallic, the bond density effect on Tg becomes systematically weaker, with a crossover at <r> = 2.3. When the more metallic Sb replaces As at <r> greater than 2.3, incipient metallicity rather than directional bond covalency apparently gains control of the physics. This leads us to an examination of the electronic conductivity and, then, semiconductor-to-metal (SC-M) transitions, with their associated thermodynamic manifestations, in relevant liquid alloys. The thermodynamic components control liquid fragility and cause fragile-to-strong transitions during cooling. We tentatively conclude that liquid state behavior in phase change materials (PCMs) is controlled by liquid state SC-M transitions that have become submerged below the liquidus surface. The analogy to supercooled water phenomenology is highlighted.

CPP 66.9 Fri 12:15 ZEU 118

Glass structure and quantum efficiency of luminescent borate glass — •A. Charlotte Rimbach[1], Bernd Ahrens[1,2], Franziska Steudel[2], and Stefan Schweizer[1,2] — [1]South Westphalia University of Applied Sciences, Luebecker Ring 2, 59494 Soest — [2]Fraunhofer Application Center for Inorganic Phosphors, Branch Lab of Fraunhofer Institute for Microstructure of Materials and Systems IMWS, Luebecker Ring 2, 59494 Soest

Luminescent glasses have gained more importance in the last decades, in particular for lasers, optical fibres, and optical amplifiers. For optical applications, borate glass is very versatile in shape and a suitable host for luminescent lanthanide ions due to its good lanthanide ion solubility. The borate glass system possesses a high transparency, low melting point as well as high mechanical, chemical, and thermal stability. Various luminescent borate glasses using boron oxide as network former and lithium oxide as network modifier are prepared. Here, the ratio between network former and network modifier determines the mechanical and chemical properties of the glass. An important parameter for the evaluation of luminescent materials is the absolute photoluminescence quantum efficiency (QE), i.e. the ratio of emitted to absorbed photons. While the ratio between network former and network modifier affects the QE only slightly, additional doping with aluminium oxide to reduce hygroscopicity results in a significant decrease in QE. Raman and Fourier transform infrared spectroscopy are used to analyze the structure of the glass network; the results are correlated with the QE measurements.

CPP 67: Focus: Topological Problems in the Physics of Polymers, Biopolymers and Fibers II (joint session BP/CPP, organized by CPP)

Time: Friday 10:15–13:00 Location: ZEU 222

CPP 67.1 Fri 10:15 ZEU 222

Mechanical properties of entwined knotted/unknotted DNA loops — •Saeed Najafi and Raffaello Potestio — MPIP, Mainz, Germany

Self-entanglement and knotting can play a crucial role in the mechanical and functional properties of bio-polymers such as DNA and RNA strands and fibers. By means of computer simulations of model DNA systems, we demonstrate that the crossing pattern of a braid of entwined DNA rings has a large impact on its structural and dynamical properties. In particular, we identify under which conditions the braid crossing pattern enforces a positive and stronger correlation between the entangled rings.

CPP 67.2 Fri 10:30 ZEU 222

Entropic interactions between two knots on a semiflexible polymer — •Stefanie Stalter, David Richard, Jonathan Siebert, and Peter Virnau — Institut für Physik, JGU Mainz Staudingerweg 7, 55128 Mainz

Two knots on a string can either be separated or intertwined and may even pass through each other. On the microscopic scale such transitions may occur spontaneously driven by thermal fluctuations and can be associated with a topological free energy barrier. In this manuscript we study the respective location of a trefoil (3_1) and a figure-of-eight (4_1) knot on a semiflexible polymer, which is parameterized to model dsDNA in physiological conditions. Two cases are considered: First, end monomers are grafted to two confining walls of varying distance. Free energy profiles and transition barriers are then compared to a subset of free chains, which contain exactly one 3_1 and one 4_1 knot. For the latter we observe a small preference to form an intertwined state, which can be associated with an effective entropic attraction.

CPP 67.3 Fri 10:45 ZEU 222

Knotted and unknotted ring polymers under shear — •Maximilian Liebetreu and Christos N. Likos — Faculty of Physics, University of Vienna, Austria

The behavior of single 3_1-knotted (trefoil) rings in a fluid under shear is compared to their unknotted ring polymer counterparts. We simulate flexible polymers of a fixed size in a thermostatted Multi-Particle Collision Dynamics (MPCD) solvent (with fixed control parameters) with Lees-Edwards boundary conditions. We primarily investigate the differences in shape parameters for 3_1-knotted and 0_1-unknotted rings in dependency of shear rate, as well as characteristics of average number of beads being part of the knot (knot size), angle between knot center of mass and first principal axis relative to the polymer's center of mass, and correlations between these quantities. We compute the relaxation time of 3_1-knotted rings and present results on their tumbling- and tank-treading dynamics. We obtain evidence suggesting that on a knotted ring, the 3_1 knot itself develops a tendency to be located near those beads closest to the orientational axis, aligned with the flow. We also show that the average knot size is decreasing with increasing shear. Preliminary findings indicate the 3_1-knotted rings responding to lower shear rates than their unknotted counterparts, and suggest a binary-state behavior for the 3_1-knotted ring under strong shear, with the knot size alternating between rather stable tight and relatively unstable delocalised configurations. Special attention is paid to the correlation between alignment angle and knot size.

Invited Talk CPP 67.4 Fri 11:00 ZEU 222

Protein Folding under Mechanical Load — •Matthias Rief — Physikdepartment der TU München, James-Franck-Str. 85748 Garching

The development of nano-mechanical tools like AFM and optical traps has made it possible to address individual biomolecules and study their response to mechanical forces. These techniques allow us to study and induce conformational changes of proteins in real time. In my talk, I will show how single molecule mechanical methods can be used to study folding of proteins. Examples will include the folding of the calcium binding protein calmodulin, as well as the folding of a protein with knotted structure.

15 min break

CPP 67.5 Fri 11:45 ZEU 222

Entropic vs Energetic stiffness in biopolymers — •Tatjana Škrbić[1], Achille Giacometti[1], Trinh Hoang[2], Artem Badasyan[3], and Rudolf Podgornik[4] — [1]University of Venice, Italy — [2]Institute of Physics, Hanoi, Vietnam — [3]University of Nova Gorica, Slovenia — [4]University of Ljubljana, Slovenia

Homopolymers form a high temperature swollen (coil) phase and a low temperature phase globular phase. The glassy nature of this ground state stems from the inability of homopolymers to reduce their entropy as temperature is decreased.

Recent attempts to introduce additional ingredients allowing the removal of this glassy ground state and hence the onset of alpha-helical and beta-sheet like structures, characteristic of proteins, will be presented. In particular, it will be shown how the introduction of an entropic stiffness breaks the spherical symmetry of the interactions and leads to the formation of protein secondary structures.

Further, the difference between this entropic stiffness and the conventional energetic stiffness characteristic of semi-flexible polymers will be pointed out, as well as the relevance of the latter for the ground state phase diagram of DNA in a bad solvent.

Finally, the relevance of the presented results for the protein design, as well as for the interpretation of experimental results on the DNA condensation, will be discussed.

References [1] T. Škrbić et al, J. Chem. Phys. (2016) [2] T. Škrbić et al, Soft Matter (2016) [3] T.X. Hoang et al, Phys. Rev. E (2015) [4] T.X. Hoang et al, J. Chem. Phys. (2014)

Invited Talk CPP 67.6 Fri 12:00 ZEU 222

All-atom simulations of folding of proteins with topologically complex native structures. — •Pietro Faccioli and Silvio a Beccara — Physics Department , Trento University, Trento, Italy

Investigating protein folding using MD remains a formidable task. Using the Anton supercomputer it is now possibile to perform folding simulations of small globular proteins, with folding times in the ms scale. On the other hand, proteins with topologically complex or even knotted native structures can take much longer to fold. Thus investigating these processes by plain MD is well beyond the reach of any present nor foreseen supercomputer.

Our group has developed an enhanced path sampling approach based on a rigorous variational approximation, which enables to simulate the folding of protein of virtually any size with folding time as long as tens of minutes using all atom force fields. This method has been first validated against the results of Anton and then applied to larger systems with increasingly complex topology. In this talk I will review our recent results concerning the folding of the smallest knotted protein and of a serpin, a large (~400 amino-acid) misfold-prone protein with a very complex native structure architecture.

In both cases we find that, in contrast to what happens to simpler globular proteins, sequence-dependent non-native interactions are playing an important role in guiding the folding process, in particular by ensuring that the native contacts are formed in the right order.

30 min panel discussion

CPP 68: Hydrogels and Microgels II

Time: Friday 10:15–13:15 Location: ZEU 260

CPP 68.1 Fri 10:15 ZEU 260

Modelling photothermal control of gold nanoparticle loaded microgel systems — •Dmitry Chigrin[1,2], Gero von Plessen[1], Ahmed Mourran[2], and Martin Möller[2,3] — [1]Institute of Physics (1A), RWTH Aachen University, Aachen, Germany — [2]DWI - Leibniz Institute for Interactive Materials, and Functional Interactive Polymers, Aachen, Germany — [3]Institute of Technical and Macromolecular Chemistry, RWTH Aachen University, Aachen, Germany

Temperature-responsive microgels can exhibit extremely large deformations due to the volume transition in response to changes in temperature. Combining photothermal materials, e.g. plasmonic nanoparticles, with microgels opens a unique opportunity to design microdynamical systems (microswimmers, microactuators, micromachines) which can be controlled all-optically. In this presentation we discuss physical modelling of gold nanoparticle loaded microgels. A description of photothermally activated microgels involves self-consistent coupling of diffusion, elasticity, heat transfer and electrodynamic models. Using simple examples we discuss how swelling/de-swelling dynamics of microgels can be controlled and guided using light.

CPP 68.2 Fri 10:30 ZEU 260

Magneto-optical and magneto-rheological properties of a physical hydrogel based on 12-hydroxystearic acid — Hajnalka Nádasi[1], Ralf Stannarius[1], Peter Salamon[2], Tamas Börzsönyi[2], and •Alexey Eremin[1] — [1]Institute of Experimental Physics, Otto von Guericke University Magdeburg, Universitätsplatz 2, 39016 Magdeburg, Germany — [2]Wiegner Research Centre for Physics, Institute for Solid State Physics and Optics, Budapest, H-1525, Hungary

We investigate magneto-responsive physical ferrogels based on 12-hydroxystearic acid in dodecane, doped with commercial magnetic nanoparticles APG 935. The gelator molecules form a hydrogen-based gel network at room temperature. The pure gels exhibit extraordinary helical filament nanostructures similar to those of the HNF(B4) liquid crystal phase formed by bent-core mesogens. The rheological behaviour of the ferrogel is found to be strongly dependent on the preparation protocol. The ferrogels prepared in a magnetic field exhibit lower storage modulus, which can be attributed to rearrangements of the magnetic particles embedded in the gel matrix. At higher shear rates, a gel-sol transition occurs. In a magnetic field, the interaction between the magnetic particles and the matrix lead to an increase of both storage and loss moduli.

The authors acknowledge the support by DFG (SPP 1681, STA 425/36-2)

CPP 68.3 Fri 10:45 ZEU 260

Structure and rheology of microgel monolayers at the water/oil interface — •Shilin Huang[1], Kornelia Gawlitza[2], Regine von Klitzing[2], Werner Steffen[1], and Günter K. Auernhammer[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität, Berlin, Strasse des 17. Juni 124, 10623 Berlin, Germany

We investigate the rheological property of microgel monolayers at the water/oil interface using passive and active microrheological methods. At low surface coverage, the microgels at the water/oil interface have a tendency to form aggregated structures (networks) with dominating elasticity. At high surface coverage the microgels form densely packed monolayers. Using microsized magnetic particles as the local rheological probes in the dense microgel monolayers, we perform in situ study of their rheolocial properties and structures. We observe four regimes where the elasticity of the microgel monolayer has different dependence on the microgel concentration at the interface. The rheological properties of the microgel monolayers are not only dependent on the concentration, but also strongly correlated with the inter-microgel distance and spacial arrangement of the microgels at the interface. Our results also show that the microgel monolayers act similar to soft glassy materials.

CPP 68.4 Fri 11:00 ZEU 260

Linear thermoresponsive acrylamid based microgels adsorbed on a surface — •Marian Cors[1], Julian Oberdisse[2], and Thomas Hellweg[1] — [1]Bielefeld University, Bielefeld, Germany — [2]Laboratoire Charles Coulomb, Université de Montpellier, Montpellier, France

A gel is a dispersed system which consists of at least two different components: a solid or flexible mesh and a fluid. If the fluid is water the gel is called a hydrogel. Microgels are gels smaller than 10 μm and can be used in a wide range of applications like drug delivery and smart surface coatings. If the microgel consists of acrylamides like N-isopropylmethacrylamide (NIPMAM) or N-n-propylacrylamid (NNPAM) as network component, they show a volume phase transition (VPT) at a certain temperature, the volume phase transition temperature (VPTT). An increase in temperature above the VPTT leads to an abrupt decrease in size and a decrease in temperature leads to an abrupt increase in size. The VPTT is specific for each monomer. To use microgels in sensors or for nanoactuators the thermoresponse has to be precise and well known. That is why we investigated microgels with a complex architecture containing NIPMAM and NNPAM. These particles show a tunable linear change in size between the two VPTTs of NNPAM (22 °C) and NIPMAM (43 °C). Furthermore, we deposited these microgels on surfaces and investigated the properties of the microgel coating. The properties of these particles (like phase transition behavior or particle size) can be adjusted by selecting specific synthesis conditions.

CPP 68.5 Fri 11:15 ZEU 260

Analysis of PDMAEMA Polymer Brushes: A TOF-SIMS Study — •Marc Thomas[1,2], Ulrich Hagemann[2,3], Steffen Franzka[2,3], Mathias Ulbricht[1,2], and Nils Hartmann[1,2,3] — [1]Chemistry Department, University of Duisburg-Essen, Germany — [2]Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Germany — [3]Interdisciplinary Center for Analytics on the Nanoscale (ICAN), University of Duisburg-Essen, Germany

Stimuli-responsive polymer brushes are widely applicable, i.e. for self-cleaning coatings, switchable adsorbers and sensors. Using controlled reaction schemes, e.g. ATRP (atom transfer radical polymerization), tailor-made ultrathin brushes can be synthesized. These brushes respond reversibly to stimuli, e.g. temperature, pH, or biomolecules within micro-/milliseconds. Hence, these brushes pose a pathway to innovative miniaturized devices. Tailoring the brushes towards bioapplications requires an insight on their inner structure without and with biomolecules. Here, TOF-SIMS has been applied to obtain three-dimensional molecular information from PDMAEMA (Poly(N,N-dimethylaminoethyl methacrylate) brushes with nm depth resolution. For varying initiator densities, the relative density of initiator prior and after the polymerization as well as the polymer chain density has been obtained. Further, the distribution of BSA (bovine serum albumin) has been examined. The TOF-SIMS experiments were complemented by XPS, AFM and fluorescence spectroscopy measurements. The results reveal the inner structure of polymer brushes of varying grafting densities without and with protein.

CPP 68.6 Fri 11:30 ZEU 260

Uptake and stability of pH-Sensitive Gold Nanoparticles (AuNPs) in Thermoresponsive Polymer Brushes — •Dikran Kesal[1], Patrick Krause[1], Marcus Trapp[2], and Regine von Klitzing[1] — [1]TU Berlin, 10623 Berlin, Germany — [2]Helmholtz Zentrum Berlin, 14109 Berlin, Germany

Polymer brushes are polymers tethered to a surface or interface by one end, which at sufficiently high grafting densities show a stretched conformation away from the surface. Many of its applications, for e.g. sensoric and catalysis, involve interaction with particles of some kind, so understanding the interactions between nanoparticles and polymer brushes is of great importance. Embedding nanoparticles, e.g. AuNPs, in polymer brushes result in nanocomposite materials with novel optical properties.

In this work, the assembly of charge switchable AuNPs inside neutral charged Poly(N-isopropylacrylamide) (PNIPAM) brushes will be discussed. The 5 nm AuNPs are capped with mercaptopropionic acid (MPA, pKa 5.5) which bears a carboxylate group and is either protonated (uncharged) or deprotonated (negatively charged) depending on the pH. While some recent efforts have been made in terms of particle uptake and distribution in weakly (PDMAEMA) and strongly

(PMETAC) charged polymers due to electrostatic interaction between particle and brush. While PNIPAM brushes are neutral charged and can only interact via H-bonding with the AuNPs, here the focus is on understanding how protonating and deprotonating of the AuNPs affect particle loading, distribution and stability in PNIPAM brushes.

15 min break

CPP 68.7 Fri 12:00 ZEU 260

Surface forces of polyelectrolyte multilayers in different growth regimes — •Heba S. Mohamad, Malte Passvogel, Annkatrin Sill, and Christiane A. Helm — Inst. of Physics, Greifswald University, D-17487 Greifswald

Interaction with the surface of polyelectrolyte multilayer films is important for many application. The films built from Poly (styrenesulfonate) (PSS) and poly (diallylmethylammonium) (PDADMA) in 0.1 Mol/L NaCl start with a parabolic growth regime. Then a transition to linear growth occurs. In the linear growth regime, there are more positive PDADMA than negative PSS monomers in the film; therefore Na^1 ions are incorporated. PDADMA and PSS terminated films in the parabolic growth regime show flat surfaces which interact purely electrostatically, as surface forces measurements with the colloid probe technique show. In the linear growth regime, PSS terminated films are also flat, but PDADMA terminated films interact by steric forces which are analysed with the Alexander-de-Gennes theory. The PDADMA chains protruding into solution are attributed to the excess PDADMA monomers within the film. We conclude that choosing the growth regime allows to control the surface interactions.

CPP 68.8 Fri 12:15 ZEU 260

Composition of polyanion mixtures influence exponential growth of polyelectrolyte multilayers — •Annkatrin Sill[1], Malte Passvogel[1], Antonia Weltmeyer[1], Olaf Soltwedel[2], Amir Azinfar[1], Peter Nestler[1], and Chrstiane A. Helm[1] — [1]Inst. of Physics, Greifswald University, Germany — [2]Physics Department, TU Munich, Germany

The exponential growth regime of polyelectrolyte multilayer films made from binary polyanion mixtures is investigated. Films were assembled by the layer-by-layer (LbL) technique using poly(stryrene sulfonate) PSS as polyanion and poly (diallyldimethylammonium) (PDADMA) as polycation and investigated with in-situ ellipsometry and neutron reflectivity. The films grow exponentially if molecular weight Mw(PSS) is below 25 kDa; no exponential film growth occurs if Mw(PSS) is above this threshold. Exponential growth is characterized by diffusion of PSS within the film; in non-exponential growth regimes PSS is immobile. The influence of PSS molecular weight distribution on exponential film growth is investigated using a PSS mixture with molecular weight below and above the threshold value. Multilayer films grow exponentially if the mole fraction of non-diffusing PSS is less than 1 %. Neutron reflectivity shows that the mole fraction of non-diffusing PSS in the film is much larger than in the preparation solution. The effect gets more pronounced with increase of the adsorption time. This finding is attributed to the irreversible adsorption of immobile PSS which replaces mobile PSS which adsorbed first.

CPP 68.9 Fri 12:30 ZEU 260

Segmental Dynamics of Spin-Labeled Poly(acrylic acid) in Polyelectrolyte Complex Coacervates Studied by CW EPR Spectroscopy — •Uwe Lappan, Brigitte Wiesner, and Ulrich Scheler — Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Straße 6, 01069 Dresden, Germany

The complex coacervation of oppositely charged polyelectrolytes has been studied by continuous wave (CW) EPR spectroscopy. The spin-label technique employs stable radicals which are covalently attached to macromolecules. Rotational dynamics of such spin labels on time scales between 10 ps and 1 μs can be characterized by basic and fast CW EPR spectroscopy. The dynamics of the spin labels is influenced by the restricted motion of the side group bearing the label and local polymer backbone motions at the point of the covalent attachment of the label. The dynamics of polyelectrolyte complexes (PECs) composed of poly(diallyldimethylammonium chloride) (PDADMAC) and poly(acrylic acid) (PAA) was studied in dependence on pH and temperature using a spin-labeled PAA as reporter molecule. All of the experimental spectra were well reproduced by simulations based on the microscopic order/macroscopic disorder (MOMD) model. It was found that the segmental mobility of the PAA in the PECs is nearly constant in the range of pH from 10 to 5 but decreases dramatically for pH values lower than 5. It has been confirmed that the dynamics in the PECs is strongly influenced by the degree of dissociation of the weak polyacid.

CPP 68.10 Fri 12:45 ZEU 260

Drug delivery by thermoresponsive polyelectrolyte complex coatings for bone healing — •Martin Müller[1,2], David Vehlow[1,2], and Birgit Urban[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Abteilung Polyelektrolyte und Dispersionen, 01069 Dresden, Germany — [2]Technische Universität Dresden, Fachrichtung Chemie und Lebensmittelchemie, 01062 Dresden, Germany

Recently, polyelectrolyte complex (PEC) particle coatings were shown to release ionic bone therapeutic drugs in sustained manner immediately after contact to buffer solutions. To trigger thermally on demand the drug release thermoresponsive PEC particle coatings based on poly(N-isopropylacrylamide-co-acrylic acid) (PNIPAM-AA) and cationic cellulose (EDAC) were fabricated. EDAC/PNIPAM-AA dispersions featured hydrodynamic radii RH=260-860 nm for T=25°C and RH=60-140 nm for T=50°C due to coil/globule transition (CGT) of PNIPAM moieties above lower critical solution temperature (LCST). Coatings of EDAC/PNIPAM-AA particles at germanium model substrates kept adhesive after buffer rinsing. FTIR spectroscopy at EDAC/PNIPAM-AA revealed significant hydrogen bonding state changes and broad phase transitions as a function of temperature as well as higher LCST values for dispersions (45°C) and coatings (50°C) compared to PNIPAM solutions (33°C). EDAC/PNIPAM-AA coatings were loaded with zoledronate (ZOL) and at T>LCST ZOL was released faster compared to T<LCST. Presumably, CGT partly compacts and defects the PEC phase enabling faster ZOL elution.

CPP 68.11 Fri 13:00 ZEU 260

Spontaneous jumping and long-lasting bouncing of solid Leidenfrost drops — •Doris Vollmer, Maxime Paven, Tadashi Kajiya, Hans-Jürgen Butt, and Jonathan Pham — MPI for Polymer Research, Mainz

The impact and rebound of liquid drops on hot, solid surfaces is of practical importance in industrial processes, such as thermal coating and spray cooling. The impact of solid spheres is also a commonly encountered event in ball milling, powder processing, and everyday activities, such as ball sports. Liquid drop and solid ball impacts are distinct from each other in terms of their mechanics. Here, we show that hydrogels display unique characteristics of both solids and liquids when heated above the Leidenfrost temperature. Using high speed video microscopy, we demonstrate that millimetric hydrogel drops jump from a hydrophilic surface upon heating and continue to bounce several times with increasing height. While elasticity dominates the mechanics of contact, evaporation supports long-lasting bouncing. This interplay between elastic and liquid properties results in intriguing dynamics, which is reflected in spontaneous jumping, long-lasting bouncing, trampolining, and the shortest contact times ever observed for water-like systems.

CPP 69: Thin Films, Nanostructures and Nanoparticles II

Time: Friday 10:15–13:00 Location: ZEU 114

CPP 69.1 Fri 10:15 ZEU 114

Shear Exfoliation of layered silica in organic solvents — •Michael Huth and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

There is a large interest in the delamination of layered silica for the production of nanocomposites. Those nanocomposites can be used for several applications, like reinforcement, flame retardant agent, or barrier applications. For all those applications, a uniform dispersion of monolayers in the nanocomposites is essential for the improvement of overall performance. In this work, layered silicaes with different intercalated molecules, so-called intercalated agents are used. Those agents change the interlayer distance between the layers forming the silica flake. The influence of those changes on the dispersion process, as well as on the morphology of the dispersed plates is investigated. The dispersions of clay are processed using a shear exfoliation in chloroform. The dispersions consist of layered silica flakes of ~ 1.5 μm length and with a thickness down to 3 nm, equivalent less than four monolayers. The obtained high aspect ratio flakes, were characterized by microscopy (TEM and AFM), UV-Vis and gravimetric measurement. The results show that high interlayer distances favor a stable dispersion of layered silicaes with a thickness of just a few monolayers.

CPP 69.2 Fri 10:30 ZEU 114

Gas permeation through free-standing carbon nanomembranes — •Petr Dementyev[1], Polina Angelova[2], Henning Vieker[2], Daniel Emmrich[1], and Armin Gölzhäuser[1] — [1]Universität Bielefeld, Fakultät für Physik, Universitätsstr. 25, Bielefeld — [2]CNM Technologies GmbH, Herforder Str. 155a, Bielefeld

Despite membranes-based gas separation can provide lower operation costs compared to distillation and sorption methods, membranes of superior permeance and selectivity are still under development. 2D materials seem to be promising in this context, as nanoporous membranes with the least thickness and no tortuosity would provide the ultimate permeation rate and could potentially work as molecular sieves.

Herein we employ a newly developed high vacuum permeation setup to study mass transport through free-standing carbon nanomembranes (CNMs). CNMs are formed out of self-assembled monolayers of molecules and are mechanically stable. Furthermore, CNMs can be fabricated on a large scale, and their properties are widely tunable depending on the preparation conditions.

Various CNMs were probed towards permeation of helium, neon, nitrogen, oxygen, argon and carbon dioxide. Mass-spectrometry detection enabled to determine the permeation rate and the membrane selectivity. Some of the samples were found to have defects with a characteristic size of 100 nm which was confirmed by helium ion microscopy. In turn, the intact samples were proved to be dense but highly selective to helium. We discuss the mechanism of gas separation as well as the origin of defects.

CPP 69.3 Fri 10:45 ZEU 114

Transfer and characterization of covalently modified large area graphene — •Felix Rösicke[1,2], Marc A. Gluba[1], Christoph Kratz[3], Timur Shaykhutdinov[3], Norbert H. Nickel[1], Jörg Rappich[1], and Karsten Hinrichs[3] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]SALSA - School of Analytical Sciences Adlershof, Berlin, Germany — [3]Leibniz - Institut für Analytische Wissenschaften - ISAS - e.V., Department Berlin, Berlin, Germany

We have investigated the electrochemical grafting of CVD grown large area graphene, as grown on copper, by p-(N-maleimido)phenyl residues from the respective diazonium salt (p (N maleimido)phenylbenzenediazonium tetrafluoroborate). The samples were characterized using Raman backscattering and infrared spectroscopic ellipsometry measurements, both prior and after transfer to a thin gold film on silicon. Optical simulations of the C=O vibrations were performed, determining the thickness of the functional layer to approximately 4 nm, showing the possibility of a lossless transfer. Furthermore, AFM-IR experiments were performed to confirm both the thickness and homogeneity of the maleimido layer. To prove the reactivity of the p-(N-maleimido)phenyl layer, the Michael addition of a thiol was monitored via IR-microscopy. Considering the variety of possible diazonium cations, this opens the possibility to the use of modified graphene as tailored modular building block for facile and specific surface functionalization.

CPP 69.4 Fri 11:00 ZEU 114

Pyrolysis of carbon nanomembranes studied by gas permeation measurements — •André Beyer, Nils Klement, Riko Korzetz, Xianghui Zhang, Berthold Völkel, and Armin Gölzhäuser — Physics of Supramolecular Systems and Surfaces, Bielefeld University, 33615 Bielefeld, Germany

Carbon nanomembranes (CNMs) from aromatic self-assembled monolayers are made by electron exposure of the molecular monolayers, resulting in cross-linked membranes which are 1 nm thick and exhibit molecular sieving characteristics in gas permeation experiments [1]. Annealing at 1200 K in vacuum transforms CNMs into nanocrystalline graphene [2, 3]. Here, this transformation process is studied by gas permeation measurements of CNMs after annealing at different intermediate temperatures in the range between 600 K and 900 K. To this end, CNMs were placed onto polydimethylsiloxane (PDMS) membranes after completion of the annealing process to determine their gas permeation characteristics with different gases (He, Ne, CO$_2$, Ar, Kr, N$_2$). A resistance model is employed to discriminate the permeation characteristics of the annealed CNMs from the PDMS support membranes [1]. It is found that a major part of the transformation process occurs at temperatures between 670 K and 770 K.

[1] M. Ai et al., Adv. Mater. 26 (2014) 3421.

[2] A. Turchanin et al., Adv. Mater. 21 (2009) 1233.

[3] A.Turchanin, et al., ACS Nano 5 (2011) 3896.

CPP 69.5 Fri 11:15 ZEU 114

Transparent Graphene Electrodes for Biomedical Applications — •Pranoti Kshirsagar[1], Thomas Chassé[3], Monika Fleischer[2], and Claus J. Burkhardt[1] — [1]NMI Natural and Medical Sciences Institute at the University of Tübingen, 72770 Reutlingen (Germany) — [2]Institute for Applied Physics and Center LISA+, Eberhard Karls University Tübingen, 72076 Tübingen (Germany) — [3]Institute of Physical and Theoretical Chemistry and Center LISA+, Eberhard Karls University Tübingen, 72076 Tübingen (Germany)

Since its isolated preparation in 2004, graphene is one of the most extensively researched materials. However, the entry of graphene into the field of biomedicine is relatively recent. Microelectrode arrays (MEAs) are often used to record the cellular activity from cells like neurons or cardiomyocytes. Au, TiN, Pt and PEDOT-CNTs are some of the electrode materials which are excellently suited for the cellular recordings. However, all these materials are opaque posing limitation for applications such as optogenetics and calcium imaging.

Here we present the development of MEAs with transparent graphene electrode and their application. 2.5 cm x 2.5 cm largely monolayer graphene is CVD grown and subsequently transferred onto the conduction lines of a MEA substrate. Detailed correlative scanning electron microscopy (SEM) and Raman spectroscopy is performed confirming the presence of graphene after each processing step. SEM is used for visualization of graphene and Raman confirms the number of layers. Graphene micro electrodes of 30 micron diameter are fabricated with this reliable process and successfully tested with cell cultures.

15 min break

CPP 69.6 Fri 11:45 ZEU 114

Patterned 2-D materials by laser ablation and self-assembly — •Daniel Rhinow[1], Natalie Freese[2], Julian Scherr[3], Andreas Terfort[3], André Beyer[2], Armin Gölzhäuser[2], and Norbert Hampp[4] — [1]Max-Planck-Institut für Biophysik, Abteilung Strukturbiologie, 60438 Frankfurt, Deutschland — [2]Universität Bielefeld, Fakultät für Physik, 33501 Bielefeld, Deutschland — [3]Goethe-Universität Frankfurt, Fachbereich Chemie, 60438 Frankfurt, Deutschland — [4]Philipps-Universität Marburg, Fachbereich Chemie, 35032 Marburg, Deutschland

Self-assembled monolayers (SAMs) of thiols on gold can be patterned using a variety of physical and chemical methods. Irradiation of SAMs on gold with a pulsed 532 nm laser beam leads to thermal desorption of thiol molecules. The gaps are filled with a second thiol SAM and a patterned SAM is obtained. Photothermal patterning of SAMs enables the fabrication of arbitrary structured monolayers with lateral dimensions in the centimetre range. We demonstrate that phothothermal desorption of aromatic thiols can be used to produce patterned two-dimensional materials. Patterned carbon nanomembranes have been analyzed by helium ion microscopy, scanning electron microscopy and photoelectron spectroscopy.

CPP 69.7 Fri 12:00 ZEU 114

Surface-Enhanced Characterization of Nanoparticle Surfaces — •Christian Kuttner[1,2], Roland P.M. Höller[1], Martin Mayer[1,2], Max J. Schnepf[1], and Andreas Fery[1,2,3] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany — [2]Cluster of Excellence Centre for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, 01062 Dresden, Germany — [3]Physical Chemistry of Polymeric Materials, Technische Universität Dresden, 01069 Dresden, Germany

We present the retrieval of molecular information at nanoparticle surfaces using surface-enhanced Raman scattering (SERS). The electric-field enhancement of the localized surface plasmon resonances (LSPRs) of noble metal nanoparticles can be exploited for the local characterization of their molecular surface near field. [1]
Consequently, we studied the nanoparticles' ligand corona in dispersion and its exchange based on the example of low-molecular-weight surfactants against high-molecular-weight proteins. [2]

[1] Höller, R.P.M. *et al.*, *ACS Nano* **2016**, *10*, 5740–5750.
[2] Tebbe, M. *et al.*, *ACS Appl. Mater. Interfaces* **2015**, *7*, 5984–5991.

CPP 69.8 Fri 12:15 ZEU 114

***In-situ* Small-angle X-ray Scattering and UV-vis spectroscopy Investigations of the Formation and Growth of Inorganic Nanoparticles by Microwave-Assisted Solvothermal Synthesis** — •Robert Wendt[1], Eike Gericke[1], Dragomir Tatchev[2], Armin Hoell[3], Markus Wollgarten[3], Simone Raoux[3], and Klaus Rademann[1] — [1]Humboldt-Universität zu Berlin, Berlin, Germany — [2]Bulgarian Academy of Sciences, Sofia, Bulgaria — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Microwave-assisted solvothermal syntheses (MWASS) have become subject of renewed fundamental interests in the preparation of crystalline and monodisperse inorganic nanoparticles (NPs). Main features of MWASS are distinguished control and exact on-line determination of pressure and temperature inside the autoclave-type reactors. The advantage is the efficient internal volumetric "in-core" heating by direct coupling of MW energy to the reaction molecules. It allows high heating rates with small thermal gradients and strongly decreased reaction times based on the Arrhenius law. This work includes innovative *in-situ* investigations of the formation and growth mechanisms of inorganic NPs by this new developed MWASS-system. It allows exact additions of precursor solution into the sealed reactor and withdrawals of colloid solution at any time. Thereby, we are able to investigate and characterize the NPs in a time-range of seconds by *in-situ* UV-Vis spectroscopy and SAXS and *ex-situ* by TEM, EELS and EXAFS. These results provide new insights in the formation and growth mechanisms.

CPP 69.9 Fri 12:30 ZEU 114

Metrology on Nascent Soot Particles from Flames by Helium Ion Microscopy — •Daniel Emmrich[1], Maurin Salamanca[2], Lena Ruwe[2], Henning Vieker[1], André Beyer[1], Katharina Kohse-Höinghaus[2], and Armin Gölzhäuser[1] — [1]Physics of Supramolecular Systems, Bielefeld University, 33615 Bielefeld, Germany — [2]Department of Chemistry, Bielefeld University, 33615 Bielefeld, Germany

Soot emissions from combustion processes are a problem for environment and health. A detailed understanding on the formation process of soot is a prerequisite for the development of strategies to reduce the emission of soot. While mature soot particles are spherical aggregates with dimensions of 20-50 nm, nascent soot particles are smaller and structurally inhomogeneous. Thus, especially the latter poses challenges in their characterization. In this study, we extracted soot particles from flames of different fuels and use helium ion microscopy (HIM) to determine size and shape of the particle down to a size of 2 nm. HIM is a scanning technique similar to scanning electron microscopy (SEM) but taking advantage from the higher mass of the helium ions. The use of helium ions in comparison to electrons in SEM enables higher contrast accompanied with high resolution, high surface sensitivity and low beam currents resulting in low sample damage. This microscope enables high throughput and high resolution to follow the growth of nascent soot particles taken at different distances from the burner surface [1, 2]. [1] M. Schenk et al., ChemPhysChem, 14, 3248 (2013) [2] M. Schenk et al., Proc Combust Inst, 35, 1879 (2015)

CPP 69.10 Fri 12:45 ZEU 114

Mean free path of slow electrons retrieved from velocity map imaging of aerosol particles — •Maximilian Goldmann[1], Bruce L. Yoder[1], Stavros Amanatidis[1], Egor Chasovskikh[1], Lukas Lang[1], Andras Bodi[2], David Luckhaus[1], and Ruth Signorell[1] — [1]Laboratorium für physikalische Chemie, ETH Zürich, 8093 Zürich — [2]Swiss Light Source, Paul Scherrer Institut, 5232 Villigen

Electron mean free paths are important quantities for a number of physico-chemical phenomena ranging from aerosol physics and chemistry to radiation damage of biological tissues. We introduce and apply a novel method to determine the electron mean free path of low energy electrons in solid and liquid materials by velocity map imaging photoelectron spectroscopy of neutral aerosol particles using vacuum ultraviolet light. We extract the electron mean free path by comparing experimental with simulated photoelectron velocity map images of aerosol particles. For the simulation, we use a detailed scattering model [1].

Experimental photoelectron spectra of potassium chloride nanoparticles [2], liquid water droplets [1], and liquid-coated nanoparticles are presented. These photoelectron images were recorded at the VUV beamline at Paul Scherrer Institute and by means of a home-built table-top laser system.

[1] R. Signorell et al., Chem. Phys. Lett. 658, 1 (2016).
[2] M. Goldmann et al., J. Chem. Phys. 142, 224304 (2015).

CPP 70: Organic Electronics and Photovoltaics V: OPV (joint session CPP/DS/HL, organized by CPP)

Time: Friday 10:15–13:15 Location: ZEU 255

CPP 70.1 Fri 10:15 ZEU 255

Non-Radiative Voltage Losses Reduce the Upper Limit of the Power Conversion Efficiency in Fullerene-Based Organic Solar Cells — •Johannes Benduhn[1], Kristofer Tvingstedt[2], Fortunato Piersimoni[3], Sascha Ullbrich[1], Dieter Neher[3], Donato Spoltore[1], and Koen Vandewal[1] — [1]IAP, TU Dresden — [2]EP VI, University of Würzburg — [3]University of Potsdam

The open-circuit voltage of organic solar cells (OSCs) is low as compared to the optical gap of the absorber molecules, indicating high energy losses per absorbed photon. These voltage losses arise only partly due to necessity of an electron transfer event to dissociate the excitons. A large part of these voltage losses is due to recombination of photo-generated charge carriers, including inevitable radiative recombination. In this work, we study the non-radiative recombination losses and we find that they increase when the energy difference between charge transfer (CT) state and ground state decreases. This behavior is in agreement with the energy-gap law for non-radiative transitions, which implies that internal conversion from CT state to ground state is facilitated by skeletal molecular vibrations. This intrinsic loss mechanism, which until now has not been thoroughly considered for OSCs, is different in its nature as compared to the commonly considered inorganic photovoltaic loss mechanisms of defect, surface, and Auger recombination. As a consequence, the theoretical upper limit for the power conversion efficiency of a single junction OSC reduces by 25% as compared to the Shockley-Queisser limit for an optimal optical gap of the main absorber between (1.45-1.65) eV.

CPP 70.2 Fri 10:30 ZEU 255

Quantifying Coupling Rate Constants of Bound Charges to the Ground State and Free Charges in Organic Semicon-

ductors — •Safa Shoaee[1], Martin Stolterfoht[1], and Ardalan Armin[2] — [1]Institute for Physics and Astronomy, University of Potsdam, Potsdam, Germany — [2]School of Mathematics and Physics, University of Queensland, Australia

Bimolecular recombination of the free charges in the donor/acceptor organic solar cells has been considered as the main loss mechanism. For very few donor/acceptor systems the bimolecular recombination rate constant is shown to be lower than what predicted by the classic Langevin model. We and others have recently shown that this suppression may originate from weaker coupling rate of the so called interfacial charge transfer states to the ground state [Burk et al. AEM 2015, Armin et al. AEM 2016]. In Particular we have shown that recombination can be 150 times less than that predicted by Langevin model, resulting in efficiencies as high as 9%, at junction > 300 nm. These studies show the importance of the kinetic constants of the charge transfer states. Recently we have developed methodology to quantify these kinetic rates as well as charge generation efficiency in organic photovoltaic systems [Stolterfoht, Shoaee et al. Nature Comm 2016, Shoaee et al. Unpublished results], as well as determining the kinetic rate constants of the charge transfer states. These are pathway towards better understanding donor acceptor solar cells and optimise their photovoltaic performance for better efficiencies.

CPP 70.3 Fri 10:45 ZEU 255

Energy losses in organic small molecule photovoltaics — •Theresa Linderl, Alexander Hofmann, Thomas Zechel, and Wolfgang Brütting — Universität Augsburg, 86135 Augsburg, Germany

One of the most important factors that limits the efficiency of organic photovoltaics is the relatively large energy loss between the optical gaps of the neat materials and the open-circuit voltage $V_{\rm OC}$. Partly, this can be explained by the energetic offset between the energy levels of the donor and acceptor material, which is often called the driving force to form the charge transfer complex. The energy of this charge transfer complex is regarded as the upper limit for $V_{\rm OC}$ at 0 K. In contrast, at room temperature $V_{\rm OC}$ is further reduced by radiative and non-radiative recombination losses.

By combining different donors with fullerene and non-fullerene acceptor materials, we have investigated the influence of interface energetics, molecular orientation and morphology on the total energy loss in organic small molecule solar cells. We find, that for proper non-fullerene acceptor materials the overall loss can be significantly reduced to about 0.6 eV, which is comparable to the best polymer solar cells.

CPP 70.4 Fri 11:00 ZEU 255

Sensitive charge transfer state spectroscopy in organic solar cells — •Martin Streiter, Alexander Wagenpfahl, and Carsten Deibel — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

The understanding of recombination mechanisms at donor–acceptor interfaces is of high importance for improving organic solar cells as the former determine both photocurrent and open circuit voltage. In order to investigate the influence of interface structure on charge transfer state recombination, we use confocal emission and excitation spectroscopy which we developed and applied to study the reorganisation energy of single molecules [1]. Sensitive measurements of both emission and excitation spectra on the timescale of seconds enable the characterisation of environmental and molecular conformational influences on dynamic spectral properties. Using this technique, we investigate the donor–acceptor charge transfer state in diluted bulk heterojunction systems. We discuss the impact of reorganisation energy and energetic disorder on the charge transfer state distribution in systems directly relevant for organic solar cells.

[1] M. Streiter, S. Krause, C. von Borczyskowski, C. Deibel, J. Phys. Chem. Lett., 7, 4281 (2016).

Invited Talk

CPP 70.5 Fri 11:15 ZEU 255

Charge transfer states for organic opto-electronics — •Koen Vandewal — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, George-Bähr-Strasse 1, 01062, Dresden, Germany

Intermolecular charge transfer (CT) states at the interface between electron-donating and electron-accepting (A) materials in organic thin films are characterized by absorption and emission bands within the optical gap of the interfacing materials. Depending on the used donor and acceptor materials, CT states can be very emissive, or generate free carriers at high yield. The former can result in rather efficient organic light emitting diodes, via thermally activated delayed fluorescence, while the latter property is exploited in organic photovoltaic devices and photodetectors. In this contribution, we will discuss the fundamental properties of CT states and link them to organic optoelectronic device performance. Furthermore, we introduce a new device concept, using an optical cavity resonance effect to boost CT absorption at photon energies below the optical gap of both donor and acceptor, enabling narrow-band, near infrared (NIR) photo-detection.

15 min break

CPP 70.6 Fri 12:00 ZEU 255

Interfacial Energetics in Organic Multi-Heterojunctions by Charge-Transfer Emission — •Christian Kästner[1], Koen Vandewal[2], Daniel A. M. Egbe[3], and Harald Hoppe[4] — [1]Institute of Thermodynamics and Fluid Mechanics, Technische Universität Ilmenau, Am Helmholtzring 1, 98693 Ilmenau, Germany — [2]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), George-Bähr-Str. 1, 01069 Dresden, Germany — [3]Linz Institute for Organic Solar Cells, Johannes Kepler University Linz, Altenbergerstr. 69, 4040 Linz, Austria — [4]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosphenweg 7a, 07743 Jena, Germany

Charge generation via exciton dissociation in organic solar cells requires donor-acceptor interfaces. Semi-crystalline phases of polymer and fullerene domains result in smaller energy gaps between the highest occupied molecular orbital and the lowest unoccupied molecular orbital as compared to the situation for amorphous phases. These molecular energy level shifts result in different interfacial charge transfer (CT) transitions depending on the disordered or ordered character of interfacing domains. In this work, a systematic variation of the order at the donor-acceptor interface was obtained via ternary blending of semi-crystalline and amorphous model polymers with a fullerene acceptor (PCBM). Using photo- and electroluminescence spectroscopy, various transition energies due to recombination across different donor-acceptor interfaces could be detected.

CPP 70.7 Fri 12:15 ZEU 255

Charge transfer recombination at planar hybrid inorganic/organic interfaces — •Ulrich Hörmann[1], Fortunato Piersimoni[1], Stefan Zeiske[1], Lukas Hoffmann[2], Thomas Riedl[2], and Dieter Neher[1] — [1]Universität Potsdam, Potsdam, Germany — [2]Bergische Universität Wuppertal, Wuppertal, Germany

The role of the intermolecular energy gap in all-organic donor/acceptor heterojunction (HJ) solar cells is well established. In the case of hybrid inorganic/organic HJs the situation is less clear. Recently, Piersimoni et al. have shown that the energy of the hybrid charge transfer (HCT) emission in electroluminescence experiments correlates with the interface energetics determined by UPS and with the open circuit voltage ($V_{\rm oc}$) of hybrid solar cells [1]. Here we focus on photovoltaic characterization of planar HJs between ZnO or SnO_x acceptor layers and different organic donor materials. Tools well established for all-organic solar cells are carefully transferred to these hybrid systems and their validity is confirmed. Reconstruction of the dark jV-curve from light intensity dependent measurement of $V_{\rm oc}$ and the short circuit current gets rid of the otherwise drastic influence of the series resistance in these devices and allows access to the ideality factor associated with the hybrid interface. Temperature dependent characterization in a carefully chosen operation regime allows the extraction of an effective energy gap, whose origin is – opposed to all-organic HJs – not completely clear, yet. With our combined analysis, we shed light on the nature of HCT states and their role for recombination at metal oxide/organic interfaces.

[1] Piersimoni et al. / Phys. Chem. Lett. 6, 500 (2015)

CPP 70.8 Fri 12:30 ZEU 255

Overcoming interfacial losses in solution-processed organic multi-junction solar cells — •Xiaoyan Du[1], Ole Lytken[1], Hans-Peter Steinrück[1], Rainer H. Fink[1], Ning Li[2], and Christoph Brabec[2] — [1]Physical Chemistry 2 and ICMM Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) Egerlandstr. 3, 91058 Erlangen, Germany — [2]Institute of Materials for Electronics and Energy Technology (i-MEET) Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) Martensstraße 7, 91058 Erlangen, Germany

We report on a systematic study of interface losses in both single- and multi-junction solar cells based on representative polymer donors and hole transporting layers (HTLs). It is found that a facile mixed HTL containing PEDOT:PSS and MoOx nanoparticles successfully overcomes the interfacial losses in both single- and multi-junction solar cells based on various active layers by reducing interface protonation, promoting better energy-level alignment, and forming a dense and smooth layer. Multi-junction solar cells with different polymers containing nitrogen atoms as the first layer and the mixed PEDOT:PSS and MoOx nanoparticles as HTL reach fill factor (FF) of over 60%, and power conversion efficiency (PCE) of over 8% [1], while the identical stack with pristine PEDOT:PSS or MoOx nanoparticles show significantly lower performance. This work is funded by the DFG within GRK 1896. [1] X. Du, et.al, Adv. Energy Mater. 2016, DOI:10.1002/aenm.201601959

CPP 70.9 Fri 12:45 ZEU 255

Following the Formation of Metal Electrodes for Organic Photovoltaics — •Franziska Löhrer[1], Volker Körstgens[1], Matthias Schwartzkopf[2], Alexander Hinz[3], Oleksandr Polonskyi[3], Thomas Strunskus[3], Franz Faupel[3], Stephan Roth[2,4], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, D-85748 Garching — [2]Deutsches Elektronensynchrotron DESY, D-22607 Hamburg — [3]CAU zu Kiel, Institut für Materialwissenschaft, D-24143 Kiel — [4]KTH, Teknikringen 56-58, SE-100 44 Stockholm

With their easy processability, high flexibility and tunable optical properties, organic photovoltaics offer a wide range of potential applications. Although based on organic materials, photovoltaic devices typically contain metal contacts due to their unrivaled electronic conductivity. These contacts have a major influence on the solar cell performance. Our work focuses on the nanostructure evolution of metal-polymer interfaces inherent in organic solar cells. We follow the morphological changes during the sputter deposition of metal electrodes onto photoactive layers using in-situ GISAXS and GIWAXS. This technique allows us to investigate the deposition process with a high spatial as well as temporal resolution. Comparing the deposition behavior of typical electrode materials (such as Au or Al) on thin films of photoactive organic materials (e.g. PTB7) helps to understand their influence on the respective photovoltaic performance.

CPP 70.10 Fri 13:00 ZEU 255

Procedures and Practices for Evaluating Thin-Film Solar Cell Stability — •Roland Rösch[1], Tobias Faber[1], Monica Lira-Cantu[2], Elizabeth von Hauff[3], Thomas Brown[4], and Harald Hoppe[1] — [1]CEEC Jena, FSU Jena — [2]ICN2, Barcelona — [3]Vrije Universiteit Amsterdam — [4]University of Rome "Tor Vergata"

Novel thin film PV technologies require an attestation of their stability in order to get ready for their qualification. In order to improve the understanding of degradation effects and how they can be prevented, stress testing under different conditions is commonly applied. By careful combination of stress factors and thorough analysis of photovoltaic parameter decaying curves, an understanding of the underlying degradation pathways can be gained. With the help of standardized and accelerated stress tests, as described in the ISOS-protocols [1], statements concerning application lifetimes can finally be made and compared among different labs. Once a photovoltaic technology has proven long lasting durability, the ultimate barrier for entering the commercial market are the IEC tests, taking a deeper look on overall safety and reliability, not only on durability. Here, the most prominent stress tests are reviewed, discussed and extended with respect to learning the most about photovoltaic device stability [2]. The most prominent outcome of this discussion an analytical determination of the *burn-in* time (tS) and furthermore the operational lifetime (tS80) and the lifetime energy yield (LEY), a newly introduced figure of merit as a measure for the energy a solar cell can produce during its lifetime. [1] Reese, SOLMAT, 95 (2011) 1253-1267 [2] Roesch, AEM, 5 (2015) 1501407

CPP 71: Frontiers of Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond

Time: Friday 10:30–13:00 Location: HSZ 02

Invited Talk CPP 71.1 Fri 10:30 HSZ 02

Going Beyond Conventional Functionals with Scaling Corrections and Pairing Fluctuations — •Weitao Yang — Duke University

Fractional fractional charges and fractional spins provide a clear analysis of the errors of commonly used functionals. We developed a scaling correction scheme by imposing the Perdew-Parr-Levy- Balduz linearity condition. Our novel scheme leads to the significantly improved description of dissociating molecules, transition-state species, and charge-transfer systems. Within many-electron theory, we have formulated the ground-state exchange-correlation energy in terms of pairing matrix linear fluctuations, opening new a channel for density functional approximations. This method has many highly desirable properties. It has minimal delocalization error with a nearly linear energy behavior for systems with fractional charges, describes van der Waals interactions similarly and thermodynamic properties significantly better than the conventional RPA, and captures the energy derivative discontinuity in strongly correlated systems. We also adopted pp-RPA to approximate the pairing matrix fluctuation and then determine excitation energies by the differences of two-electron addition/removal energies. This approach captures all types of interesting excitations: single and double excitations are described accurately, Rydberg excitations are in good agreement with experimental data and CT excitations display correct 1/R dependence.

Invited Talk CPP 71.2 Fri 11:00 HSZ 02

Multi-reference density functional theory — •Andreas Savin — Laboratoire de Chimie Théorique, CNRS and UPMC, Univ. Paris VI, Sorbonne University, Paris, France

It is sometimes said that there is no multi-reference density functional theory. The talk presents a personal viewpoint, and will focus on the following points. 1) There are many ways to introduce multi-determinant wave functions into density functional theory. 2) Several variants have been successfully explored. 3) Difficulties inherent to approximations (both for wave functions and density functionals) persist, but can be attenuated.

Invited Talk CPP 71.3 Fri 11:30 HSZ 02

Density functionals from machine learning — •Kieron Burke — UC Irvine

Machine learning is spreading to all aspects of our lives. A particular method, kernel ridge regression, has proven very useful for fitting and interpolating in high-dimensional spaces.

Several years ago, in collaboration with the group of Klaus-Robert Muller in computer science at TU Berlin, we demonstrated how to construct a machine-learned density functional on a simple toy problem, non-interacting fermions in a box. We showed both its successes and limitations. We have continued to develop this method (PRL, 2012).

I will report on two recent works. In the first (arXiv:1609.02815), we construct the non-interacting kinetic energy functional for small molecules in 3D using a basis. We avoid the challenge of finding functional derivatives by learning the potential to density map directly, thereby bypassing the need to solve the Kohn-Sham equations.

In the second, we learn the interacting functional directly for the first time. In 1D, we model chains of H atoms of different length, and learn F[n] itself, from highly accurate DMRG calculations. With a novel choice of basis for the densities, we are able to learn the functional to chemical accuracy in the thermodynamic limit (arXiv:1609.03705).

Invited Talk CPP 71.4 Fri 12:00 HSZ 02

Taming Memory-Dependence in Time-Dependent Density Functional Theory — •Neepa Maitra — Hunter College of the City University of New York

The exact exchange-correlation functional of time-dependent density functional theory (TDDFT) is known to depend on the history of the densities and the initial states, a dependence which is ignored in almost all of the calculations today that use an adiabatic approximation. The lack of this dependence can sometimes lead to drastically incorrect predictions of the dynamics, as has been shown in several examples recently. We present here a new approach to developing functional approximations that breaks free of the adiabatic approximation, and test the resulting approximations on a number of model systems.

Invited Talk CPP 71.5 Fri 12:30 HSZ 02

Quantum Embedding Theories — •Fred Manby — School of Chemistry, University of Bristol, Cantock's Close, Bristol, BS8 1TS, UK

Issues of accuracy in density functional theory can be addressed by making more accurate methods (like coupled-cluster theory) more efficient; or by making density functional approximations more accurate. Efforts in both directions are underway in our group, but in this talk I will focus on a third possibility, namely the development of quantum-mechnical multiscale models that enable the use of a high-accuracy method in a small, physically important region coupled to density-functional theory (or other low-cost methods) to describe the molecular environment.