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Fachverband Chemische Physik und Polymerphysik (CPP)

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Overview of Invited Talks and Sessions

(Lecture rooms H37, H40, H42, and H51; Poster B2)

Invited Talks

CPP 3.1	Mon	9:30–10:00	H40	**Orientation effects in polymer networks** — •Vladimir Toshchevikov
CPP 6.1	Mon	9:30–10:00	H51	**Dynamics of thermosensitive core-shell dumbbells as analyzed by rheo-SANS** — •Matthias Ballauff
CPP 6.8	Mon	11:45–12:15	H51	**Percolation in colloidal model systems** — •Tanja Schilling, Hugues Meyer, Mohit Dixit, Mark Miller, Paul van der Schoot
CPP 8.1	Mon	15:00–15:30	H40	**The role of nonlinearities and kinetics at phase transitions in stimuli-responsive polymer solutions and hydrogels** — •Martine Philipp, Winfried Petry, Peter Müller-Buschbaum
CPP 17.1	Tue	9:30–10:00	H40	**Molecular Dynamics Simulations of Compacted Polyelectrolyte Complexes** — •Diddo Diddens, Jörg Baschnagel, Albert Johner
CPP 20.1	Tue	9:30–10:00	H51	**Photoinduced Surface Patterning in Azo-Polymers: How Can Supramolecular Functionalization Strategies Serve Us?** — •Arri Priimägi
CPP 20.6	Tue	11:15–11:45	H51	**Plasmon coupling in self-assembled colloidal monolayers** — •Matthias Karg
CPP 23.2	Tue	14:15–14:45	H40	**Challenges and opportunities of nanostructured block copolymer membranes for lithium-ion batteries** — •Ezzeldin Metwalli, Majid Rasool, Simon Brunner, Peter Müller-Buschbaum
CPP 25.1	Tue	14:00–14:30	H51	**Plasmonic heating brings dynamic control of microgel shape and locomotion** — •Ahmed Mourran, Hang Zhang, Martin Moeller
CPP 32.1	Wed	9:30–10:00	H37	**Towards 100% efficient OLEDs using thermally activated delayed fluorescence; how does the spin conversion work** — •Andrew Monkman, Marc Etherington, Paul Klein, David Graves, Przemyslaw Data, Paloma dos Santos Lays, Roberto Nobuyasu, Youhei Tacked, Fernando Dias
CPP 32.6	Wed	11:15–11:45	H37	**Effects of charge and exciton diffusion on triplet-polaron quenching and triplet-triplet annihilation in disordered organic semiconductors** — •Reinder Coehoorn, Harm van Eersel, Le Zhang, Peter Bobbert, Rene Janssen
CPP 33.3	Wed	10:00–10:30	H40	**Quasi-elastic neutron scattering study of an ionic liquid confined in nanoporous carbon** — Mark Busch, Tommy Hofmann, Boris Dyatkin, Yuri Gogotsi, Alexei Kornyshev, Jan Embs, Bernhard Frick, •Patrick Huber
CPP 34.1	Wed	9:30–10:00	H42	**Polymer crystallization and nucleation: New insights from fast scanning calorimetry** — •Christoph Schick, Evgeny Zhuravlev, René Androsch
CPP 35.6	Wed	11:00–11:30	H51	**The extraordinary mechanical properties of spider silk and it's molecular foundation** — •Friedrich Kremer, Markus Anton, Periklis Papadopoulos, Roxana Figuli, Wilhelm Kossack
CPP 39.1	Wed	15:00–15:30	H37	**The Nature of the 'Triplet Pair State' in Singlet Exciton Fission.** — •Jenny Clark, Andrew Musser, Chaw Keong Yong, Daniel Polak

CPP 40.3	Wed	15:30–16:00	H40	**Competing oligonucleotide macromolecules: binding preferences instead of a ménage a trois** — •Albrecht Ott
CPP 41.1	Wed	16:00–16:30	H42	**From holes to drops to toroids: Transcription of surface patterns into 3D-morphologies by dewetting** — •Günter Reiter, Samer Al Akhrass, Laurant Vonna
CPP 42.5	Wed	16:00–16:30	H51	**A coarse-grained model for DNA: dynamics of self-assembling biological systems and nanostructures.** — •Ard Louis
CPP 42.8	Wed	17:15–17:45	H51	**Principle of Maximum Caliber and its application in biology** — •Kingshuk Ghosh
CPP 42.9	Wed	17:45–18:15	H51	**Coarse-graining of conservative and non-conservative interactions in molecular liquids** — •Nico van der Vegt
CPP 48.1	Thu	9:30–10:00	H37	**It is water what matters: THz absorption spectroscopy as a new tool to study solvation dynamics** — •Martina Havenith
CPP 48.3	Thu	10:15–10:45	H37	**Dielectric and diffusional aspects of hydration water** — •Roland Netz, Matej Kanduc
CPP 48.5	Thu	11:15–11:45	H37	**Neutron scattering clarifies the behaviour of water in cells** — •Giuseppe Zaccai
CPP 48.7	Thu	12:00–12:30	H37	**Controlling Water Evaporation: self-assembly at air/liquid interfaces** — •Emma Sparr, Kevin Roger
CPP 49.1	Thu	9:30–10:00	H40	**Patterned organic ferroelectric memory diodes by solution micromolding** — •Paul Blom, Thomas Lenz, Simon Benneckendorf, Kamal Asadi, Dago de Leeuw
CPP 50.1	Thu	9:30–10:00	H42	**Provoking liquids to dewet and to slide: About concave drops and hungry droplets** — •Karin Jacobs
CPP 52.1	Thu	9:30–10:00	H51	**Synthesis of 2D polymers** — •Dieter A. Schlüter
CPP 52.2	Thu	10:00–10:30	H51	**Carbon nanomembranes as a platform for engineering of functional 2D materials** — •Andrey Turchanin
CPP 60.1	Thu	15:00–15:30	H51	**Evolution of mono- and bilayer graphene in chemical vapor deposition and the thinnest feasible porous membranes for ultimate mass transport** — •Hyung Gyu Park
CPP 61.1	Thu	16:15–16:45	H51	**Tuning of ordering in colloidal suspensions confined in thin films** — Sebastian Schön, Yan Zeng, Sabine Klapp, •Regine von Klitzing

Tutorials

CPP 1.1	Sun	16:00–16:50	H18	**Perovskite photovoltaics: Synthesis, structure and device architecture** — •Pablo Docampo
CPP 1.2	Sun	16:50–17:40	H18	**Charge Carrier Generation and Recombination in Organic and Perovskite Solar Cells** — •Andreas Baumann
CPP 1.3	Sun	17:40–18:30	H18	**The electronic structure in hybrid perovskite layers and devices** — •Selina Olthof

Invited talks of the joint symposium SYHP

See SYHP for the full program of the symposium.

SYHP 1.1	Mon	9:30–10:00	H1	**Perovskite Semiconductors: Opportunities and Challenges for Photovoltaic Materials Design** — •David B. Mitzi
SYHP 1.2	Mon	10:00–10:30	H1	**Perovskite Solar Cells: A new Paradigm in Photovoltaics** — •Mohammad Nazeeruddin
SYHP 1.3	Mon	10:30–11:00	H1	**Charge-Carrier Diffusion and Radiative Efficiencies in Hybrid Metal Halide Perovskites** — •Laura Herz
SYHP 1.4	Mon	11:15–11:45	H1	**Photovoltage losses in perovskite solar cells** — •Kristofer Tvingsted
SYHP 1.5	Mon	11:45–12:15	H1	**Computational screening of perovskite solar energy materials** — •Karsten W. Jacobsen

Invited talks of the joint symposium SYAD

See SYAD for the full program of the symposium.

SYAD 1.1	Thu	15:00–15:30	H15	**Phenomenology of Collective Chemotaxis in Artificial and Living Active Matter** — •Ramin Golestanian
SYAD 1.2	Thu	15:30–16:00	H15	**First-passage times of Markovian and non Markovian random walks in confinement** — •raphael Voituriez
SYAD 1.3	Thu	16:00–16:30	H15	**Cytoskeleton organization as an optimized, spatially inhomogeneous intermittent search strategy** — •Heiko Rieger, Yannick Schröder, Karsten Schwarz
SYAD 1.4	Thu	16:45–17:15	H15	**Ergodicity violation and ageing in living biological cells** — •Ralf Metzler
SYAD 1.5	Thu	17:15–17:45	H15	**Anomalous diffusion within cells** — Sarah Klein, •Cecile Appert-Rolland, Ludger Santen

Sessions

CPP 1.1–1.3	Sun	16:00–18:30	H18	**Tutorial: Hybrid and Perovskite Photovoltaics (CPP/DF/DS/HL, organized by CPP)**
CPP 2.1–2.5	Mon	9:30–12:15	H1	**Symposium SYHP: Fundamentals of Hybrid and Perovskite Photovoltaics (CPP/DS/DF/HL, organized by CPP)**
CPP 3.1–3.9	Mon	9:30–12:15	H40	**Polymer Networks and Elastomers**
CPP 4.1–4.10	Mon	9:30–12:15	H41	**Nanoparticles, Nanocrystals and Composites I**
CPP 5.1–5.6	Mon	9:30–11:00	H45	**Colloids and Complex Fluids I (joint session BP/CPP/DY, organized by BP)**
CPP 6.1–6.11	Mon	9:30–13:00	H51	**Colloids and Complex Fluids II (joint session BP/CPP/DY, organized by CPP)**
CPP 7.1–7.9	Mon	15:00–17:30	H38	**Hybrid and Perovskite Photovoltaics I (joint session CPP/DF/DS/HL, organized by CPP)**
CPP 8.1–8.9	Mon	15:00–17:45	H40	**Hydrogels and Microgels**
CPP 9.1–9.6	Mon	15:00–16:30	H41	**Nanoparticles, Nanocrystals and Composites II**
CPP 10.1–10.11	Mon	15:00–18:00	H42	**Colloids and Complex Fluids III (joint session BP/CPP/DY, organized by CPP)**
CPP 11.1–11.24	Mon	18:15–21:00	Poster B2	**Poster: Hybrid and Perovskite Photovoltaics**
CPP 12.1–12.18	Mon	18:15–21:00	Poster B2	**Poster: Colloids and Complex Fluids**
CPP 13.1–13.14	Mon	18:15–21:00	Poster B2	**Poster: Nanoparticles, Nanocrystals and Composites**
CPP 14.1–14.7	Mon	18:15–21:00	Poster B2	**Poster: Polymer Networks and Elastomers, Hydrogels, Soft Robotics**
CPP 15.1–15.8	Mon	18:15–21:00	Poster B2	**Poster: Functional Polymer Hybrids**
CPP 16.1–16.2	Tue	9:30–10:30	H3	**High Efficiency Photovoltaics (joint session AKE/CPP, organized by AKE)**
CPP 17.1–17.10	Tue	9:30–12:30	H40	**Polyelectrolytes**
CPP 18.1–18.12	Tue	9:30–12:45	H42	**Molecular Electronics and Photonics**
CPP 19.1–19.12	Tue	9:30–13:00	H47	**Microswimmers (joint session BP/CPP/DY, organized by DY)**
CPP 20.1–20.10	Tue	9:30–12:45	H51	**Focus: Functional Polymer Hybrids I**
CPP 21.1–21.8	Tue	10:45–13:00	H37	**Hybrid and Perovskite Photovoltaics II (joint session CPP/DF/DS/HL, organized by CPP)**
CPP 22.1–22.6	Tue	14:00–15:30	H37	**Organic Electronics and Photovoltaics I (CPP/DS/HL/O, organized by CPP)**
CPP 23.1–23.5	Tue	14:00–15:30	H40	**Charged Soft Matter**
CPP 24.1–24.5	Tue	14:00–15:15	H46	**Complex Fluids and Colloids IV (joint session BP/CPP/DY, organized by DY)**
CPP 25.1–25.6	Tue	14:00–16:00	H51	**Focus: Functional Polymer Hybrids II**
CPP 26.1–26.9	Tue	18:15–21:00	Poster B2	**Poster: Charged Soft Matter, Polyelectrolytes, Ionic Liquids**
CPP 27.1–27.8	Tue	18:15–21:00	Poster B2	**Poster: Soft Matter Dynamics / Glasses**
CPP 28.1–28.6	Tue	18:15–21:00	Poster B2	**Poster: Computational Physics of Soft Matter**
CPP 29.1–29.8	Tue	18:15–21:00	Poster B2	**Poster: Crystallization, Nucleation, Self Assembly**
CPP 30.1–30.37	Tue	18:15–21:00	Poster B2	**Poster: Organic Electronics and Photovoltaics**

CPP 31.1–31.8	Wed	9:30–11:45	H11	**Hybrid and Perovskite Photovoltaics III (joint session CPP/DF/DS/HL, organized by DS)**
CPP 32.1–32.10	Wed	9:30–12:45	H37	**Focus: Triplet States in Organic Optoelectronics I**
CPP 33.1–33.11	Wed	9:30–12:45	H40	**Ionic Liquids and Water**
CPP 34.1–34.9	Wed	9:30–12:15	H42	**Crystallization, Nucleation, Self Assembly I (joint session CPP/DY, organized by CPP)**
CPP 35.1–35.12	Wed	9:30–13:00	H51	**Activated and Glassy Dynamics of Soft Matter (joint session CPP/DY, organized by CPP)**
CPP 36.1–36.11	Wed	10:00–13:00	H47	**Complex Fluids and Colloids V (joint session BP/CPP/DY, organized by DY)**
CPP 37.1–37.9	Wed	10:30–13:00	S054	**Organic-Inorganic Systems II: Energy Level Alignment (organized by O)**
CPP 38.1–38.12	Wed	14:45–18:30	H2	**Organic Photovoltaics and Electronics (joint session CPP/HL, organized by HL)**
CPP 39.1–39.5	Wed	15:00–16:30	H37	**Focus: Triplet States in Organic Optoelectronics II**
CPP 40.1–40.11	Wed	15:00–18:15	H40	**Biomaterials and Biopolymers I (joint session BP/CPP/MM, organized by CPP)**
CPP 41.1–41.8	Wed	16:00–18:30	H42	**Crystallization, Nucleation, Self Assembly II (joint session CPP/DY, organized by CPP)**
CPP 42.1–42.9	Wed	15:00–18:15	H51	**Focus: Multiscale Simulations for Soft Matter: The Challenge of Dynamics (joint session CPP/DY, organized by CPP)**
CPP 43.1–43.11	Wed	18:15–21:00	Poster B2	**Poster: The Physics of Water Interactions with Biological Matter**
CPP 44.1–44.9	Wed	18:15–21:00	Poster B2	**Poster: Biomaterials and Biopolymers**
CPP 45.1–45.9	Wed	18:15–21:00	Poster B2	**Poster: Two Dimensional Functional Materials**
CPP 46.1–46.14	Wed	18:15–21:00	Poster B2	**Poster: Wetting, Nano- and Microfluidics**
CPP 47.1–47.20	Wed	18:15–21:00	Poster B2	**Poster: Interfaces and Thin Films**
CPP 48.1–48.8	Thu	9:30–12:45	H37	**Focus: The Physics of Water Interactions with Biological Matter (joint session BP/CPP, organized by CPP)**
CPP 49.1–49.11	Thu	9:30–12:45	H40	**Organic Electronics and Photovoltaics II (joint session CPP/DS/HL/O, organized by CPP)**
CPP 50.1–50.11	Thu	9:30–12:45	H42	**Wetting, Nano- and Microfluidics I (joint session CPP/DY, organized by CPP)**
CPP 51.1–51.12	Thu	9:30–13:00	H48	**Glasses (joint session CPP/DY, organized by DY)**
CPP 52.1–52.9	Thu	9:30–12:30	H51	**Focus: Two Dimensional Functional Materials I**
CPP 53.1–53.5	Thu	11:45–13:00	H52	**Biomaterials and Biopolymers II (joint session BP/CPP/MM, organized by MM)**
CPP 54.1–54.13	Thu	14:45–18:30	H2	**Hybrid and Perovskite Photovoltaics IV (joint session CPP/DF/DS/HL, organized by HL)**
CPP 55.1–55.5	Thu	15:00–17:45	H15	**Symposium SYAD: Anomalous Diffusion in Complex Environments (BP/CPP/DY, organized by BP)**
CPP 56.1–56.11	Thu	15:00–18:00	S051	**Organic-Inorganic Systems III: Electronic Structure (organized by O)**
CPP 57.1–57.13	Thu	15:00–18:30	H40	**Polymer Dynamics and Rheology (joint session CPP/DY, organized by CPP)**
CPP 58.1–58.7	Thu	15:00–16:45	H42	**Wetting, Nano- and Microfluidics II (joint session CPP/DY, organized by CPP)**
CPP 59.1–59.5	Thu	15:00–16:15	H45	**Biomaterials and Biopolymers III (joint session BP/CPP/MM, organized by BP)**
CPP 60.1–60.3	Thu	15:00–16:00	H51	**Focus: Two Dimensional Functional Materials II**
CPP 61.1–61.7	Thu	16:15–18:15	H51	**Interfaces and Thin Films I (joint session CPP/DY, organized by CPP)**
CPP 62.1–62.9	Fri	9:30–12:00	H40	**Organic Electronics and Photovoltaics III (joint session CPP/DS/HL/O, organized by CPP)**
CPP 63.1–63.9	Fri	9:30–12:00	H51	**Interfaces and Thin Films II (joint session CPP/DY, organized by CPP)**

Annual General Meeting of the Chemical and Polymer Physics Division

Donnerstag 19:00–19:30 H51

- Bericht
- Posterpreis (gestiftet von Asylum Research)
- Wahl stv. Sprecher

CPP 1: Tutorial: Hybrid and Perovskite Photovoltaics (CPP/DF/DS/HL, organized by CPP)

Organizers: Lukas Schmidt-Mende (Universität Konstanz), Vladimir Dyakonov (Universität Würzburg) and Christoph Lienau (Universität Oldenburg)

Tremendous progress has been achieved in the performance of hybrid solar cells, with efficiencies now exceeding 20 % for devices based on organometallic halide perovskites. Aim of this tutorial is to introduce this topic of perovskite solar cells to prepare for the following symposium (SYHP) and allow vivid scientific discussions. A description of current state-of-the-art device fabrication methods and solar cell architectures will be given and their role on the device performance explained. The device physics will be discussed and charge carrier generation and recombination mechanisms in perovskite films explained and compared to other material systems. Additionally the important role of electronic structure of the different layers in hybrid perovskite will be covered.

Time: Sunday 16:00–18:30 Location: H18

Tutorial CPP 1.1 Sun 16:00 H18
Perovskite photovoltaics: Synthesis, structure and device architecture — •Pablo Docampo — LMU Munich, Germany

Recently, organic-inorganic hybrid perovskites have been proven to be excellent photovoltaic materials, exhibiting outstanding light absorption, high carrier mobility and facile solution processability. Besides the manufacturing low costs of perovskite thin-films, the power conversion efficiencies demonstrated for this class of materials is already at the same level as poly-crystalline silicon and other thin film photovoltaic technologies. The pursuit of efficiency in the field of metal halide perovskite solar cells has been achieved mainly through the improvement to perovskite deposition processing and optimization of the device architecture.

In this tutorial I will focus on three topics. Firstly, the evolution of the device architecture, starting from sensitized mesoscopic solar cells to planar heterojunction devices employing organic contacts. Secondly, the commonly employed perovskite deposition techniques with special emphasis on the morphological quality of the prepared perovskite films. Thirdly, the perovskite structure and its stability both towards moisture and other factors such as UV-light, temperature and atmosphere. I will link these different aspects with device performance characteristics and introduce recent developments in the field towards surmounting the challenges the technology is currently facing from a materials point of view.

Tutorial CPP 1.2 Sun 16:50 H18
Charge Carrier Generation and Recombination in Organic and Perovskite Solar Cells — •Andreas Baumann — Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), Magdalene-Schoch-Str. 3, D-97074 Würzburg

The new star on the photovoltaic (PV) horizon, are the so called organometal halide perovskite solar cells. This new kind of thin-film PV technology has experienced a tremendous, yet not seen increase in power conversion efficiency (PCE) compared to other types of PV technologies. Up to now the solar cell efficiency on lab scale could be improved from 3.8% in 2008 to above 20% in 2015 being already competitive with commercially available PV technologies. Especially this boost in PCE values has attracted attention of many researchers from all different PV research fields. Thereby, perovskite PV is one of the most promising thin film PV technologies regarding low-cost manufacturing combined with high PCE. However, the working principle of these solar cells is yet not completely understood and is strongly discussed in literature. Phenomena, such as the often observed anomalous hysteresis in the current-voltage characteristics or the giant dielectric constant and its impact on charge carrier generation and recombination are highly debated topics with so far different given possible explanations.

In this tutorial, the processes of charge carrier generation and recombination in perovskite solar cells will be highlighted and compared to those in well studied organic solar cells. Thereby, the aim is to give an overview of the published data on these processes in order to present the current status of research.

Tutorial CPP 1.3 Sun 17:40 H18
The electronic structure in hybrid perovskite layers and devices — •Selina Olthof — University of Cologne, Institute for Physical Chemistry, Luxemburger Straße 116, 50939 Köln, Germany

The performance of optoelectronic devices strongly depends on the appropriate energetic alignment of the participating transport levels which directly influence the charge transport through the different layers. In order to optimize these interfaces in a non-trial-and-error fashion, one needs to know the conduction band minimum and valence band maximum of the perovskites to be able to select ideal transport layers as well as contact materials. While commonly vacuum level alignment is assumed at the interface to the substrate, this is actually rarely found in devices. Interfacial states, interface dipoles, and band bending can (and do) significantly alter the energy level landscape.

In this tutorial I will discuss the electronic structure of perovskites and introduce common measurement techniques that can shed a light on their energetic properties as well as the interface alignment relevant for devices. Combining reports from literature with our own recent results on the versatile electronic nature of this material I will elucidate the interplay between electronic structure and overall device performance.

CPP 2: Symposium SYHP: Fundamentals of Hybrid and Perovskite Photovoltaics (CPP/DS/DF/HL, organized by CPP)

Time: Monday 9:30–12:15 Location: H1

Invited Talk CPP 2.1 Mon 9:30 H1
Perovskite Semiconductors: Opportunities and Challenges for Photovoltaic Materials Design — •David B. Mitzi — Duke University, Edmund T. Pratt Jr. School of Engineering, Durham, NC 27708-0300 USA

Organic-inorganic and related halide-based perovskites (e.g., those based on Pb halide frameworks) have attracted substantial recent interest for solar cell and other optoelectronic technologies, because of the large optical absorption coefficients, high carrier mobilities, long minority carrier lifetimes, and relatively benign defects and grain boundaries. Indeed, these materials have enabled an unprecedented rapid improvement in photovoltaic (PV) performance to levels above 20% power conversion efficiency. Despite the great promise, challenges for the current generation of PV materials include replacing lead with more environmentally benign metals, improving PV device stability (moisture, UV and air) and controlling hysteresis. This talk will explore beyond the current focus on three-dimensional (3-D) lead(II)-based perovskites, to highlight the outstanding structural, chemical and electronic flexibility of the perovskite family. Particular focus will be afforded to systems in which divalent lead is replaced with other metal cations exhibiting a lone pair of electrons, such as Sn, Bi and Sb, since these systems share some of the beneficial electronic structure characteristics of the Pb-based systems. Further discovery within the perovskite structural and chemical space may offer prospects to solve the current technological challenges for perovskite PV and yield important opportunities for energy materials design.

Invited Talk CPP 2.2 Mon 10:00 H1

Perovskite Solar Cells: A new Paradigm in Photovoltaics — •Mohammad Nazeeruddin — EPFL, GMF, Sion Switzerland

Perovskite solar cells exhibited significant leapfrog in efficiency due to a broad absorption, high optical absorption coefficient, very low exciton binding energy, long carrier diffusion lengths, efficient charge collection, and very high open circuit potential similar to III-IV semiconductors. Unlike silicon solar cells, perovskite solar cells can be developed a variety of low-temperature solution process from inexpensive raw materials. By engineering compositional ratio of perovskite absorber, film formation using anti-solvent, and interface engineering of charge transport materials a remarkable power conversion efficiency of over 21% has been demonstrated, highlighting the unique photovoltaic properties of perovskite materials. In this talk, we present the current progress in perovskite solar cells, various deposition methods for perovskite absorbing layer, synthesis and characterization of novel hole transporting materials, and highlight crucial challenges and prospects

Invited Talk CPP 2.3 Mon 10:30 H1

Charge-Carrier Diffusion and Radiative Efficiencies in Hybrid Metal Halide Perovskites — •Laura Herz — University of Oxford, Oxford, UK

Hybrid metal halide perovskites (stoichiometry AMX$_3$) have recently emerged as low-cost active materials in PV cells with power conversion efficiencies in excess of 20%. In addition, hybrid perovskites show prospects for applications in low-cost light-emitting diodes and lasers.

Here we discuss how parameters essential for photovoltaic operation, such as charge carrier recombination and diffusion lengths are altered with substitutions of the organic A cation (e.g. methylammonium versus formamidinium), the metal M cation (e.g. Pb^{2+} or Sn^{2+}) and the halide X anion (I versus Br). We analyze distinct charge-carrier recombination mechanisms, such as trap-mediated, bi-molecular (electron-hole) and Auger recombination, which show different dependences on composition and temperature.

We use these insights to predict charge-carrier diffusion lengths and radiative efficiencies in the limit of ultra-low trap-related recombination, which could potentially be reached through further advances in material processing. We find that for hybrid lead iodide perovskites with typical charge-carrier mobilities of $\sim$30cm^2/(Vs), charge-carrier diffusion lengths under solar irradiation are unlikely to exceed $\sim$10μm even if all trap-related recombination is eliminated. We further show that if high radiative efficiencies are to be obtained for intermediate charge-carrier densities ($n\sim10^{14}$cm^{-3}), trap-related recombination lifetimes have to exceed microseconds.

15 min. break.

Invited Talk CPP 2.4 Mon 11:15 H1

Photovoltage losses in perovskite solar cells — •Kristofer Tvingsted — Experimental Physics VI, Julius Maximilians Universität, Würzburg, Germany

Perovskite PVs have reached significant power conversion efficiency in a very short time period. Apart from providing a rather high photocurrent, they also retain a comparatively high open circuit voltage (VOC). The VOC of most solar cells is however far from its potential upper limit due to charge carrier recombination of various types, whose origin must be accurately determined. Herein, I summarize what we have learned about these photovoltage losses by studying the radiative part of recombination in Perovskites. By accurate determination of the present solar cells radiative efficiency, that is their ability to emit light, we conclude how far the solar cells are from their own thermodynamic upper limit and further, how they relate to a reference OPV cell. We evaluate the carrier density dependence of the radiative efficiency and associate it to the ideality factor, which in itself represents a uniform figure of merit for the dominant type of recombination. We show that, as the perovskite steady state photoluminescence is strong at open circuit conditions, but substantially quenched only at short circuit, they perform in this respect just as an ideal solar cell should do, and also very different from most OPVs or DSSC cells studied so far. Substantially improving the radiative efficiency to increase the open circuit voltage is a promising route to put these new photovoltaic converters in efficiency parity with the best inorganic counterparts.

Invited Talk CPP 2.5 Mon 11:45 H1

Computational screening of perovskite solar energy materials — •Karsten W. Jacobsen — CAMD, Dept. of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

In the talk I shall describe computational efforts to idenfity new materials for efficient light absorption with particular focus on materials in the perovskite structure and water splitting. The materials have to obey a number of criteria in order to work for light absorption and water splitting depending on the particular design of the device. We consider in particular stability, appropriate bandgap and bandstructure for visible light absorption, and an adequate line-up of band edges to the water redox potential. We also identify descriptors to determine defect-sensitivity of the materials.

We have considered several classes of materials with most emphasis on the cubic perovskite structure and derivatives like double perovskites and layered perovskites (Ruddlesden-Popper and Dion-Jacobson phases) with anions O, N, F, or S. Also a range of Sn and Pb based organic and inorganic perovskites have been considered with different combinations of the anions I, Br, and Cl. The possibilities of band gap tuning using atomic-level heterostructures or strain will also be touched upon.

I shall finally mention presently available open databases of relevance for energy materials including the Computational Materials Repository (https://cmr.fysik.dtu.dk) where the discussed data are made publicly available.

CPP 3: Polymer Networks and Elastomers

Time: Monday 9:30–12:15 Location: H40

Invited Talk CPP 3.1 Mon 9:30 H40

Orientation effects in polymer networks — •Vladimir Toshchevikov — Leibniz-Institut für Polymerforschung Dresden e.V.

Crosslinked polymer networks remain a subject of extensive investigations due to their importance for technical applications and everyday life. Mechanical properties of these materials are determined by the change of conformations of network strands and by reorientation of chain segments under external stimuli. Incorporation of functional moieties, which can form the orientation order under external stimuli, into polymer networks opens up fascinating possibilities for creation of novel stimuli-sensitive smart materials. The present overview deals with recent theoretical developments to describe the influence of the orientation order on the mechanical properties of polymer networks. In particular, effects of the orientation order, which appears in liquid-crystalline networks [1] and in functional crosslinked polymers under mechanical [2] or electromagnetic fields [3], on the shape and on the static and dynamic moduli are discussed. The Gaussian approach for describing the statistics and mechanical properties of polymer networks is verified. [1] V. Toshchevikov et al. Macromolecules 42 (2009), 3417. [2] V. Toshchevikov et al. Macromol. Theory Simul. 19 (2010), 195. [3] V. Toshchevikov et al. J. Phys. Chem. B 116 (2012), 913; 118 (2014) 12297.

CPP 3.2 Mon 10:00 H40

Development of a new micro-structure based model for the stress-strain response of filler reinforced elastomers including temperature and rate-dependence — •Jan Plagge and Manfred Klüppel — DIK e.V., Hannover, Germany

A newly developed physical material model is presented, which was built on the main assumptions of the Dynamic Flocculation Model (DFM), but includes the stress-softening via the breakdown of highly stressed polymer-filler domains under load. The polymer-response is modeled with the non-affine tube model. Key parameters can be identified with exponents derived from percolation theory describing the cluster size distribution of fillers. Set stress and hysteresis are introduced via a continuous reaggregation mechanism, completely characterized by a critical stress parameter. This is implemented with a convolution-like memory kernel. Modeled stress-strain response is in perfect agreement with experiments. The critical stress parameter was predicted to be dependent of temperature and deformation rate by means of Kramers escape rate. This is confirmed for a wide range of temperatures and speeds by a fit to multihysteresis measurements carried out in a heat chamber. Fitting parameters reveal that the mechanism responsible for hysteresis and set stress takes place on the nanometer scale with energies of roughly 100 kJ/mol, possibly rearrangement of primary filler particles. To conclude, the newly developed model reproduces all major rubber characteristics with a small set of physically motivated parameters, making it a promising option to further understand the complex polymer-filler interplay.

CPP 3.3 Mon 10:15 H40

Morphology and Mechanical Properties of reinforced and crosslinked Polymer Blends containing EPDM — •Christoph Gögelein[1], John Beelen[2], Martin van Duin[2], Dina Gabriel[3], Alexander Karbach[3], and Brigitte Mosbach-Wetzka[4] — [1]Lanxess Deutschland GmbH — [2]Lanxess Elastomers B.V. — [3]Currenta GmbH & Co. OHG — [4]Bayer Technology Services GmbH

Due to stepwise improvements in polymer processing and recent catalyst developments, new Ethylene-Propylene-Diene-Monomer (EPDM) polymers of very high molar mass have recently been synthesized. These terpolymers exhibit up to date unseen strong mechanical properties, especially at elevated temperatures. In the present study, we investigate the dynamic-mechanical properties of certain crosslinked polymer blends containing EPDM reinforced with carbon black with respect to a significant increase of crack growth resistance and the fatigue lifetime without deteriorating the excellent heat stability of EPDM-based elastomers. Applications such as engine mounts, vibration isolation applications, exhaust mounts, and suspension bushings can benefit from the advantage of the saturated polymer backbone of EPDM, the strength and resilience of high molar mass EPDM, and the compounding techniques shown in this paper.

CPP 3.4 Mon 10:30 H40

Shape-memory polymer networks on the basis of high-density polyethylene — •Oleksandr Dolynchuk[1], Igor Kolesov[2,3], Hans-Joachim Radusch[2,3], and Jens-Uwe Sommer[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, D-01069 Dresden, Germany — [2]Martin Luther University Halle-Wittenberg, Center of Engineering Sciences, D-06099 Hale (Saale), Germany — [3]Polymer Service GmbH Merseburg, D-06217 Merseburg, Germany

Shape-memory (SM) polymers lead to many applications, in particular, as stimuli-responsive sensors and actuators. Polyethylene is considered as a promising SM material due to suitable thermal and mechanical properties, low costs and highly developed production. A theory of two-way invertible SME was developed and allowed calculation of the free energy change of high-density polyethylene (HDPE) drawn under constant load σ and cooled down below crystallization temperature. The free energy ΔF was assumed to consist of three terms: ΔF of transferring links from the amorphous to crystalline region, surface free energies, and the entropy change in the amorphous subchains. The analysis of ΔF predicted the possible morphology and orientation of crystallites generated at cooling. Experimentally determined crystallinity, size and orientation of the crystals formed in HDPE under different σ were compared with theoretical predictions got by modeling the two-way SME in HDPE. All qualitative and quantitative characteristics of the two-way SME, the experimental curves of temperature dependent strain as well as the features of generated crystalline structures are in good accordance with the results of our theoretical analysis.

15 min. break

CPP 3.5 Mon 11:00 H40

Characterization of damage mechanisms in elastomers under constraint load by x-ray investigations — •Konrad Schneider — Leibniz-Institut für Polymerforschung Dresden, Deutschland

Under conditions of use very different loading situations are applied to elastomers, mainly multiaxial loading with superimposed hydrostatic tension. The load can be applied steadily as well as cyclically. Equally diverse is the damage behaviour. First steps of damage under different conditions were investigated by x-ray scattering as well as computer tomography and discussed with respect to the damage criterion.

CPP 3.6 Mon 11:15 H40

Electric- and magnetic field responsive soft materials — •Miklos Zrinyi — Semmelweis University, Budapest, Hungary

Electric-, and magnetic field sensitive polymer gels and elastomers are soft smart materials whose elastic- and thermodynamic properties are strong function of the field strength imposed upon them. Colloidal (nano-) particles with special electric and magnetic properties are built into flexible polymer matrix. The particles couple the shape of the gel (or elastomer) to the external fields. Shape distortion occurs instantaneously and disappears abruptly when electric- or magnetic field is applied or removed, respectively. Giant deformation effect, field controlled elastic modulus, non-homogeneous deformation and quick response to magnetic- and electric field open new opportunities for using such materials for various applications. The development of smart polymer composites that show spinning in static uniform field will also be presented. The rotating disk acts like micro sized motors with tuneable angular frequency.

CPP 3.7 Mon 11:30 H40

Dynamic moduli of anisotropic magneto-sensitive elastomers — •Dmytro Ivaneyko, Vladimir Toshchevikov, and Marina Saphiannikova — Leibniz-Institut für Polymerforschung Dresden e.V.

The dynamic mechanical behavior of anisotropic magneto-sensitive elastomers (MSEs) with chain-like or plane-like distributions of magnetic particles is investigated in a low-frequency regime under a uniform external magnetic field. By this study we continue our previous work [1], in which a coarse-grained network model was proposed for description of dynamic mechanical behavior of isotropic MSEs. The average positions of magnetic particles are distributed on the sites of tetragonal lattice. The lattice anisotropy is defined by the ratio α of average distances between neighboring particles along and perpendicular to the symmetry axis: $\alpha = \langle r_{\parallel} \rangle / \langle r_{\perp} \rangle$. Equations of motion for magnetic particles take into account the influence of the elastic network and magnetic interactions between the particles under external magnetic field. It is shown that the relaxation spectrum depends on the anisotropy parameter α. The shear dynamic moduli G' and G'' of anisotropic MSEs are calculated for different geometries of application of the oscillating shear strain with respect to the magnetic field H, applied along the symmetry axis of the MSE.

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

CPP 3.8 Mon 11:45 H40

Microstructural Study of SiO2 Coated Spherical Polyelectrolyte Brushes and Hollow Silica Nanoparticles as Observed by Small-Angle X-Ray Scattering — •Haoya Han[1,2], Li Li[1], Xuhong Guo[1], and Regine v. Klitzing[2] — [1]East China University of Science and Technology, Shanghai, PR China — [2]Technical University of Berlin, Berlin, Germany

Organic-inorganic core-shell silica nanoparticles and silica hollow spheres with a porous morphology and tailored structure have received many attentions due to their versatile characteristics such as non-toxicity, biocompatibility and high mechanical strength. Here nanosized spherical polyelectrolyte brushes were successfully used as templates to synthesize monodisperse silica-coated core-shell nanospheres and hollow silica nanospheres. In order to better understand the formation mechanism of silica layer onto the brush layer and the structural details, the formed particles were systematically characterized by SAXS in combination with DLS, TEM, etc. The electron density of the outer silica layer was found higher than the inner silica layer from the SAXS fitting model. Core-shell microgel nanoparticles with polystyrene cores and crosslinked shell were further used as templates. The net-shape structure of the crosslinked shell hindered the free silica nanoparticle from going inside the brush layer. These results could promote better designs of core-shell silica nanospheres and hollow silica nanospheres, which should be ideal candidates for promising applications in drug delivery, catalysis and functional materials.

CPP 3.9 Mon 12:00 H40

Probing Polyethylene Glycol Elasticity by Single Molecule Force Spectroscopy and Molecular Dynamic Simulation — •Susanne Liese[1], Manuel Gensler[2], Stefanie Krysiak[3], Andreas Achazi[4], Beate Paulus[4], Thorsten Hugel[5], Jürgen P. Rabe[2], and Roland R. Netz[1] — [1]Freie Universität Berlin, Fachbereich Physik — [2]Humboldt-Universität zu Berlin, Department of Physics — [3]Technische Universität München, Physik Department — [4]Freie Universität Berlin, Fachbereich Chemie — [5]Universität Freiburg, Institute of Physical Chemistry

Polyethylene glycol (PEG) is a water soluble, non-toxic and very flexible polymer, which is widely used in medical and chemical applications. We investigate the elastic properties of PEG in a multi-scale approach based on a combination of ab-initio calculations, molecular dynamic simulations and single molecule force spectroscopy. A detailed analysis of the force-extension relation shows, that the entropy remains almost constant, if the polymer is stretched, which can be explained by a combination of chain stretching and conformational changes of single PEG-monomers. Our findings challenge the basic notion of polymer science, according to which polymers are entropic springs, which react to stretching with a loss of conformational entropy. Generalizing our results might be of great importance to other water soluble systems as well.

CPP 4: Nanoparticles, Nanocrystals and Composites I

Time: Monday 9:30–12:15 Location: H41

CPP 4.1 Mon 9:30 H41

Protein-Assisted Assembly of Highly Modular Plasmonic Core/Satellite Nanoclusters — •Roland Höller[1,2], Martin Dulle[3], Sabrina Thomä[2], Martin Mayer[1,2], Stephan Förster[3], Andreas Fery[1,2], Christian Kuttner[1,2], and Munish Chanana[2,4] — [1]Nanostructured Materials, Leibniz Institute of Polymer Research, 01069 Dresden, Germany — [2]Physical Chemistry II, University of Bayreuth, 95440 Bayreuth, Germany — [3]Physical Chemistry I, University of Bayreuth, 95440 Bayreuth, Germany — [4]Institute of Building Materials, ETH Zürich, 8093, Zürich, Switzerland

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. The highly modular bottom-up fabrication of colloidally stable nanoclusters was shown for homo- and heterometallic core/satellite combinations, with variable sizes of the building blocks, using different proteins. A precise characterization of the morphology of such core/satellite nanoclusters 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. Roland P. M. Höller *et al.*, **2015** (submitted).

CPP 4.2 Mon 9:45 H41

Assembly of metal-oxide nanoparticles directed by nanodomain orientation in block copolymer thin films — •Ezzeldin Metwalli[1], Yuan Yao[1], Jean-Francois Moulin[2], Matthias Opel[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Helmholtz Zentrum Geesthacht, Institut für Werkstoffforschung, MLZ, 85748 Garching, Germany — [3]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany

Both, parallel and perforated lamella morphologies of hybrid thin films [1-2] composed of maghemite nanoparticles (NPs) and PSd-b-PBMA diblock copolymer (DBC) were investigated. A systematic identification of NP arrangements within the nanostructured DBC films was obtained at different film depths using TOF-GISANS. An enrichment of NPs at the solid interface for both morphologies was observed. The dispersion stability of the PS-coated NPs in the nanostructured DBC films depends not only on the NP size but also on the orientation of the PS nanodomains. The laterally 2D confined PS domains in the perforated lamella initiate an aggregation of NPs at a lower NP concentration compared with 1D parallel lamella morphology. The potential applications in relation to medical instrumentation and magnetic sensors are highly feasible for both morphologies based on the superparamagnetic behavior of the fabricated nanocomposite films, proven with a superconducting quantum interference device magnetometer. [1] Metwalli et al., ChemPhysChem 15, 2236 (2014) [2] Y. Yao et al., ACS Appl. Mater. Interfaces 7, 13080 (2015)

CPP 4.3 Mon 10:00 H41

Fast and Slow Ligand Exchange at the Surface of Colloidal Gold Nanoparticles — •Björn Braunschweig, Rebecca Dinkel, and Wolfgang Peukert — Institute of Particle Technology (LFG), FAU Erlangen-Nürnberg, Cauerstrasse 4, 981058 Erlangen, Germany

Applications of gold nanoparticles often demand that the particle's ligand shell is modified after particle formation. Obviously, there is a great need for a molecular understanding of this process which is often not accessible in situ. Here, we have applied second-harmonic light scattering (SHS) to investigate the ligand exchange at the surface of colloidal gold nanoparticles in situ and in real time. We demonstrate that the ligand exchange at the surface of citrate-covered Au nanoparticles with 3-mercapto-1-propanesulfonate (MPS) must be described by a fast (<100 s) and a slow reaction process (<23 min) which can be attributed to MPS adsorption on low- and high-coordinated Au surface sites. Using a modified Langmuir isotherm, the average Gibbs free energy of adsorption ΔG (-46 kJ/mol) and the surface coverage Γ ($\approx$3.5 μmol/m^2) for MPS on Au nanoparticles were determined. The latter was found to be much smaller compared to planar gold surfaces which points to co-adsorption of MPS with citrate on high-coordinated sites, i.e. Au terraces. On more reactive low-coordinated Au sites, i.e. edge sites, citrate is easily replaced by MPS. In fact, we find that a substantial portion (49 %) of the surface-adsorbed MPS is present on these low-coordinated sites.

CPP 4.4 Mon 10:15 H41

Tailoring the Physicochemical Properties of Protein-Coated Gold Nanoparticles — •Jonas Schubert[1], Inna Dewald[2], Olga Isakin[2], Tobias Kraus[3], and Munish Chanana[4] — [1]Leibniz Institute of Polymer Research Dresden, 01069 Dresden, Germany — [2]Physical Chemistry II, University of Bayreuth, 95447 Bayreuth, Germany — [3]INM Leibniz-Institut for New Materials, 66123 Saarbrücken, Germany — [4]Institute of Building Materials (IfB), ETH Zurich, 8093 Zurich, Switzerland

The investigation of the behavior of nanoparticles in the environment begins with the detection of their physicochemical properties. It has up to now not been successful to connect their properties with their behavior because of the undefined adsorption of proteins onto the surface of the nanoparticles, which changes their properties drastically. One approach to circumvent this is to generate a defined protein corona. In this work, we present gold nanoparticles successfully coated with a variety of proteins, which differ in their physicochemical properties (MW, pI). These properties and the environmental conditions (pH, ionic strength) determine the colloidal stability of the nanoparticles during and after the protein adsorption in a certain pH range. Eventually, the physicochemical properties of the successfully coated NPs can be tailored by the choice of protein, the coating pH and the purification pH.

Dewald, I.; Isakin, O.; Schubert, J.; Kraus, T.; Chanana, M., J. Phys. Chem. C, 2015, 119, 25482-25492.

CPP 4.5 Mon 10:30 H41

Halloysites stabilized Pickering-emulsions: Is this the way to green chemistry? — •Dmitrij Stehl[1], Regine von Klitzing[1], Yuri Lvov[2], Tobias Pogrzeba[1], Marcel Schmidt[1], Reinhard Schomäker[1], Lena Hohl[3], Matthias Kraume[3], Joachim Koetz[4], Tina Skale[5], and Anja Drews[5] — [1]TU-Berlin, Straße des 17 Juni 124, 10623 Berlin — [2]Louisiana Tech University, 911 Hergot Ave, Ruston, LA 71272, USA — [3]TU-Berlin, Frauenhoferstr. 33-36, 10587 Berlin — [4]Universität Potsdam, Karl-Liebknecht-Straße 24-25, 14476 Potsdam — [5]HTW Berlin, Wilhelminenhofstr. 75 A, 12459 Berlin

Pickering-emulsions (PEs) are particle-stabilized emulsions. In the combination with Halloysites as stabilizing nanoparticles, PEs fulfil the qualifications of green chemistry and open up new industrial possibilities. Halloysites are multiwall, inorganic tubes with negative charges at the outer surface and positive charges at the inner surface. In this study, the hydroformylation of long chained olefins (1-Dodecene) in PEs was used as a model system, to prove the catalytic power of Halloysites. The water phase contains the homogeneous catalyst and the oil phase (1-Dodecene) is simultaneous the reactant. After the hydroformylation the expensive rhodium-catalyst can be easily separated from the product (Tridecanal) and can be reused. The effect of different parameters such as concentration of the Halloysites, energy input by the PE-fabrication, water/oil ratio and the reaction parameters were analyzed. Furthermore, we study the essential interfacial interactions between water, oil and Halloysites. In order to control the emulsion properties the Halloysites were partially hydrophobized.

CPP 4.6 Mon 10:45 H41

Lifetime-encoded Microparticles — •Daniel Kage[1], Katrin Hoffmann[1], Wolfgang Göhde[2], Thomas Thiele[3], Uwe Schedler[3], and Ute Resch-Genger[1] — [1]Federal Institute for Materials Research and Testing (BAM), Richard-Willstätter-Str. 11, 12489 Berlin — [2]Quantum Analysis GmbH, Mendelstr. 17, 48149 Münster — [3]PolyAn GmbH, Rudolf-Baschant-Straße 2, 13086 Berlin

Analytical methods require efficient and versatile strategies to measure an increasing number of analytes that can be used in conjunction with established platforms like flow cytometry. Spectral multiplexing suffers from problems such as spectral crosstalk and often requires different excitation light sources increasing instrumentation costs [1]. Thus, the number of distinguishable reporters with intensity-based barcodes is limited. An alternative can be lifetime encoding for discrimination of fluorophores based on their fluorescence decay kinetics [2].

We report on the suitability of μm-sized polymer particles stained with organic dyes for lifetime encoding. These dyes are excitable at a standard laser diode wavelength and detectable within a single spectral window. For lifetime-based discrimination, these dyes display sufficiently different luminescence decay kinetics. We present the spectroscopic properties of these beads and address challenges like the limited number of detectable photons in a flow for the reliable discrimination. These studies are expected to pave the road to new applications of fluorescence lifetime multiplexing for time-domain flow cytometry.

1.*Hoffmann, K., et al., ACS Nano, 2013. 7(8): p. 6674-84. 2.*Cao, R., et al., Opt Express, 2013. 21(12): p. 14816-31.

15 min. break

CPP 4.7 Mon 11:15 H41

Reversible switching between self-assembled nanoribbons and nanotubes — •Asad Jamal[1,2], Philippe Mesini[3], and Günter Reiter[1,2] — [1]Physikalisches Institut und — [2]Freiburger Materialforschungszentrum, Albert-Ludwigs-Universität Freiburg, 79104 Freiburg, Germany — [3]Institut Charles Sadron, 23 rue du Loess BP 84047, 67034 Strasbourg Cedex 2, France

The self-assembly of achiral 3,5-bis-(5-hexylcarbamoylpentyloxy)-benzoic acid decyl ester (BHPB-10) molecules in solution and on substrate was investigated as a function of solvent quality. Tubular structures nanotubes with diameters of ca. 30 nm were favoured in solvents having weak interactions with the molecules (cyclohexane) while in solvents with comparatively strong molecule-solvent interactions (cyclohexanone) 12 nm wide nanoribbons were formed. Both structures were several micrometers long. A switching from nanoribbons to nanotubes was observed during solvent vapour annealing in cyclohexane vapour. Nanotubes could be switched back into nanoribbons by destroying the hydrogen bonding between BHPB-10 molecules via exposure to cyclohexanone. Atomic force microscope (AFM) revealed that nanoribbons first switched to helical twisted nanosheets which were subsequently transformed into tubular structures. Thus, tuning the interactions between BHPB-10 with the quality of the solvent, we were able to form nanoribbons, which can turn into helical twisted nanosheets or nanotubes but also to reversible switch between nanoribbons and nanotubes.

CPP 4.8 Mon 11:30 H41

Oxidative etching of silver nanowires for improvement of structural integrity — •Egon Steeg[1], Frank Polzer[1], Holm Kirmse[1], Yan Qiao[1], Jürgen P. Rabe[1,2], and Stefan Kirstein[1] — [1]Department of Physics, Humboldt-Universität zu Berlin — [2]IRIS Adlershof, Humboldt-Universität zu Berlin

Silver nanowires with diameter of 6.5 nm are grown within tubular J-aggregates by reduction of silver ions. The nanowire growth starts with small isolated crystallites within the tubular aggregate that grow into pieces of wires that finally coalesce into continuous wires that homogeneously fill the template. This growth continues due to remaining silver ions within solution. The resulting crystals are wire-like, but are inhomogeneous and non-uniform in diameter. Addition of NaCl allows precipitation of the remaining silver ions in form of AgCl at defined times stabilizing the structure of the wires. The influence of oxygen is critical for this process, since the silver can be oxidized by oxygen in the solution with the chloride acting as a ligand due to oxidative etching. This etching is most effective at silver structures that contain defects or twin boundaries. The selective etching efficiency allows removing the parts of the wires that have lower structural integrity which leaves pieces with length of several hundred nanometers. This allows us not only to produce well-defined silver nanowires but to preserve their morphology in solution for weeks.

CPP 4.9 Mon 11:45 H41

Enhanced Dispersion and Alignment of Carbon Nanotubes by a High Molar Mass Amphiphilic Block Copolymer — •Matthias M. L. Arras, Roy Zitzmann, Bojia He, and Klaus D. Jandt — Chair of Materials Science (CMS), Otto-Schott-Institut für Materialforschung, Friedrich-Schiller-Universität, Jena, Germany

In this contribution multi-wall carbon nanotubes (MWCNTs) were simultaneously dispersed *and* aligned in a nanocomposite by using a high molar mass amphiphilic block copolymer (HMMABCP) matrix. HMMABCPs are promising because they are blendable with homopolymers of technically relevant molar masses. The hypotheses were tested that a HMMABCP can (i) disperse MWCNTs (ii) by a mechanism similar to low molar mass BCPs and (iii) be melt-drawn to align the MWCNTs while maintaining the degree of dispersion. The dispersion of MWCNTs within poly(styrene)-*block*-poly(2-vinylpyridine) (PS-*b*-P2VP) ($\bar{M}_w \approx 500\,\mathrm{kg\,mol^{-1}}$) and its homopolymers (control) in non-selective and selective solvents were investigated. PS-*b*-P2VP greatly improved the MWCNT dispersion which was long-term stable. The dispersion mechanism was identified as BCP micelle mediated steric stabilization. A melt-drawn MWCNT/PS-*b*-P2VP nanocomposite film showed a high degree of MWCNT dispersion *and* alignment. In comparison to a similarly processed MWCNT/poly(ethylene) nanocomposite film, the MWCNT dispersion in PS-*b*-P2VP was strongly enhanced. This contribution highlights the advantages of an intrinsically dispersive matrix which may facilitate the future application of functional nanocomposites.

CPP 4.10 Mon 12:00 H41

Dynamics and interfaces in functional polymer nanocomposites — •Ulrich Scheler — Leibniz-Institut für Polymerforschung Dresden e.V.

Nanoparticles from hydroxyapatite (HAp) and layered double hydroxides (LDH) have been investigated using solid-state NMR. 27Al NMR provides a local probe for the interface of the nanoparticles and the modifications applied to enhance to compatibility with the polymer matrix. The coordination and the local symmetry manifested in the quadrupolar coupling constant is monitored. Dedicated solid-state NMR experiments permit the selective excitation of the protons in the Hap particles. Spin diffusion from there transfers the magnetization to the nearby protons in the polymer matrix. Thus distance-dependent solid-state NMR spectroscopy becomes feasible, allowing the investigation of structure and local mobility of the polymers in contact with the inorganic filler compared to the bulk material, showing reduced polymer segment motion in the vicinity of the the particles. Additional dynamic information is available from EPR using spin-labelled polyelectrolytes in multilayers covering the nanoparticles.

CPP 5: Colloids and Complex Fluids I (joint session BP/CPP/DY, organized by BP)

Joint session with CPP and DY organized by BP.

Time: Monday 9:30–11:00 Location: H45

CPP 5.1 Mon 9:30 H45

Intracellular microfluidics to probe the role of hydrodynamic flows in embryonic cell polarization — Matthäus Mittasch[1], •Peter Gross[2], Stephan Grill[2], and Moritz Kreysing[1] — [1]MPI-CBG, Dresden, Germany — [2]Biotechnolgy Center, TU Dresden, Dresden, Germany

A hallmark of embryogenesis is the development of spatial structure.

This process is orchestrated by gene regulatory networks coupled to physical transport mechanisms. Particularly, it was suggested that the polarization of the egg cell of the nematode worm Caenorhabditis elegans, prior to asymmetric cell division, relies on interaction of two protein networks (PAR proteins) coupled to active cortical flows. However, it remains a challenge to perturb intracellular fluid mechanics to demonstrate the causal role of hydrodynamic flows in embryogenesis. Towards this end, we exploited thermo-viscous pumping (Weinert & Braun, J. appl. Phys. 2008) in order to dynamically control hydrodynamic flows inside of living embryos. Specifically, well-defined flow patterns were generated on sub- and cellular length-scales with velocities exceeding wild-type flows significantly, without affecting the biological integrity of the embryo. By application of externally-induced flows we depleted membrane-bound PAR proteins locally, suggesting that hydrodynamic flows are essential to load PAR proteins at the posterior pole. Furthermore, we perform rescue experiments in a non-polarizing embryo, by which the omitted wild-type flow will be applied externally to test if the PAR polarity can be restored artificially.

CPP 5.2 Mon 9:45 H45

Phase behavior of dense lysozyme solutions — •Julian Schulze[1], Johannes Möller[2], Michael Paulus[1], Julia Nase[1], Metin Tolan[1], and Roland Winter[3] — [1]Fakultät Physik/Delta, Technische Universität Dortmund,44221 Dortmund ,Germany — [2]ESRF - The European Synchrotron, 38043 Grenoble, France — [3]Fakultät für Chemie und Chemische Biologie, Technische Universität Dortmund, 44221 Dortmund, Germany

In previous studies, small-angle X-ray scattering (SAXS) in combination with liquid-state theoretical approaches and DLVO theory was used to study the intermolecular interaction potential V(r) of lysozyme solutions under the influence of varying environmental conditions such as protein concentration c, temperature T, and pressure p. While the repulsive Coulomb term of the DLVO potential remains almost constant as a function of p, the depth of the attractive part, J(p), exhibits a non-monotonic p-dependence with a minimum at about 2 kbar at constant T. Adding 0.5 M NaCl leads to more prominent short range interactions, especially at high c and low T, and the homogeneous protein solution becomes turbid due to formation of a metastable liquid-liquid phase separation (LLPS) region, where lysozyme forms small droplets of high concentration within the more dilute liquid phase. At elevated pressures, this l-l phase separation is suppressed, but due to the non-monotonic behavior of J(p), a further pressure increase leads to a re-entrant LLPS regime. In this contribution, we will discuss the phase behavior of lysozyme as a function of c, p, and T.

CPP 5.3 Mon 10:00 H45

Demixing and Ripening in Gradient Systems — •Christoph Weber[1], Chiu Fan Lee[2] und Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Department of Bioengineering, Imperial College, London

Ostwald ripening in homogeneous mixtures is described by the Lifshitz-Slyozov theory. It captures the phenomenon of smaller droplets that shrink, while larger ones grow. This process is driven by a difference in the Laplace pressures between the drops. Recently, liquid-like drops have been reported in living cells, which ripen in a gradient of a regulating protein component. This protein is known to affect the phase separation properties along the gradient such that drops dissolve at one and grow at the opposite side of the cell. An open question is how an inhomogeneous background affects the ripening law in contrast to the homogeneous Lifshitz-Slyozov theory.

To this end we analytically derived the corresponding growth law using a mean field theory. We find that there is a gradient of supersaturation that leads to a drift and an inhomogeneous growth of drops. The latter gives rise to a dissolution boundary that moves through the system leaving droplets only at one side of the system.

Using our mean field approach to describe the interactions between multiple drops we discover that a larger gradient of supersaturation not necessarily implies a faster ripening. Instead, droplets can be spatially sorted in size leading an arrest of the ripening dynamics for large times until homogeneous Ostwald-ripening sets in again.

CPP 5.4 Mon 10:15 H45

New analysis method for passive microrheology — •kengo nishi[1], maria l. kilfoil[2], christoph f. schmidt[1], and fred c. macKintosh[3] — [1]Georg-August-Universität Göttingen, Göttingen, Germany — [2]University of Massachusetts, Amherst, USA — [3]Vrije Universiteit, Amsterdam, Netherland

Passive microrheology is an experimental technique used to measure the mechanical response of materials from the fluctuations of micron-sized beads embedded in the medium. Microrheology is well suited to study rheological properties of materials that are difficult to obtain in larger amounts and also of materials inside of single cells. In one common approach, one uses the fluctuation-dissipation theorem to obtain the imaginary part of the material response function from the power spectral density of bead displacement fluctuations, while the real part of the response function is calculated using a Kramers-Kronig integral. The high-frequency cut-off of this integral strongly affects the real part of the response function in the high frequency region. Here, we discuss how to obtain more accurate values of the real part of the response function by an alternative method using autocorrelation functions.

CPP 5.5 Mon 10:30 H45

How to regulate droplet position in a heterogeneous chemical environment? — •Samuel Krüger[1,2], Christoph A. Weber[1], Jens-Uwe Sommer[2,3], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Leibniz Institute of Polymer Research Dresden e.V., Dresden — [3]Technische Universität Dresden, Institute of Theoretical Physics, Dresden, Germany

Cells contain chemical components that are not separated from the cytoplasm by a membrane. An example are P-granules in the C. elegans embryo. They are liquid-like structures, that form droplets. They consist of RNA and proteins that are segregated spontanuously from the cytoplasm and are known to play a role in the specification of germ cells. During asymmetric cell division, P granules are segregated to one side of the cell. This segregation is guided by a spatial concentration gradient of the protein Mex-5. We simplify the multicomponent nature of the cytoplasm with a ternary model: The P granule material, the solvent (cytoplasm), and a regulator corresponding to Mex-5. Using this model we aim to understand the physical principles controlling the droplet position in a simplified scenario, where an external potential establishes the regulator gradient. We use the Flory-Huggins mean field theory and calculate the equilibrium solutions by minimizing the free energy functional. There are two equilibrium states. Droplets either localize at high external potential or low external potential. Changing the interaction between the regulator and the solvent we find that the free energy exhibits a kink indicating that the transition between both states being a discontinuous phase transition.

CPP 5.6 Mon 10:45 H45

Finding descriptive features for the characterization of the coarsening dynamics of three dimensional foams — •Jonas Dittmann[1], Anja Eggert[2], Martina Lambertus[1], Jannika Dombrowski[3], Alexander Rack[4], and Simon Zabler[1,2] — [1]Lehrstuhl für Rötngenmikroskopie, Fakultät für Physik und Astronomie, Universität Würzburg, Germany — [2]Fraunhofer EZRT, Fürth, Germany — [3]Wissenschaftszentrum Weihenstephan, Technische Universität München, Germany — [4]European Synchrotron Radiation Facility (ESRF), Grenoble, France

Understanding the coarsening behavior of foams is essential for their deliberate design. The coarsening theories by Lifshitz, Slyozov and Wagner (LSW) as well as Glazier provide concise coarsening models with descriptive parameters that may enable systematic studies on the effects of different foam constituents.

Wet polydisperse beta-Lactoglobulin foam was imaged by fast synchrotron micro computed tomography over a period of 15 minutes in intervals of 2 to 5 minutes. The growth behavior of about 2×10^5 pores is individually observed and statistically analyzed as a function of pore radius as well as number of neighboring pores.

The three-dimensional analog of von Neumann's law by Glazier is confirmed as a fitting empirical description of the mean coarsening behavior, whereby the critical number of neighbors discriminating between shrinkage and growth is found to be 13.2 ± 5.5. Qualitative features of LSW theory are observed as well: the pore's growth rate increases with their size and a critical radius can be identified.

CPP 6: Colloids and Complex Fluids II (joint session BP/CPP/DY, organized by CPP)

Time: Monday 9:30–13:00 Location: H51

Invited Talk CPP 6.1 Mon 9:30 H51

Dynamics of thermosensitive core-shell dumbbells as analyzed by rheo-SANS — •Matthias Ballauff — Helmholtz-Zentrum Berlin

We present a study of the dynamics of dumbbell-shaped colloids. The thermosensitive dumbbell-shaped microgels consist of a solid polystyrene core and a thermosensitive shell of cross-linked poly(N-isopropylacrylamide). These colloidal particles are nearly monodisperse as shown by cryogenic transmission electron microscopy. The aspect ratio L* defined by the ratio of the center distance L to the diameter D can be varied between 0.24 and 0.3. The effective volume fraction can be varied by temperature and high volume fractions can be achieved easily because of the thermosensitive shell [1]. We observe the formation of a plastic crystal in these suspensions about of volume fraction of 0.5 as predicted by theory. This is shown from rheological evidence and by the Bragg-reflections of the crystals. For higher volume fraction a glassy state is formed. Moreover, oscillatory experiments in the linear viscoelastic regime and flow curves up to volume fractions of nearly 0.7 have been obtained. Recent studies based on a combination of rheoSANS experiments and BD-simulations revealed the formation of a novel, partially oriented phase formed by dumbbells under shear. All data demonstrate that these particles present a novel model system for the study of the rheology of slightly anisotropic particles.

[1] F. Chu, et al., Macromol. Rapid Comm. 33 (2012) 1042.

CPP 6.2 Mon 10:00 H51

Phase diagram of polydisperse colloidal dispersions — •Preecha Kiatkirakajorn[1], Joaquim Li[1], Bernard Cabane[2], Franck Artzner[3], Robert Botet[4], and Lucas Goehring[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Götingen, Germany — [2]LCMD, CNRS UMR 8231, ESPCI, 10 rue Vauquelin, 75231 Paris Cedex 05, France — [3]Institut de Physique, CNRS UMR 6626, Univ Rennes, 35042 Rennes, France — [4]Physique des Solides, CNRS UMR 8502, Univ Paris-Sud, F-91405 Orsay, France

Polydisperse colloidal dispersions have been predicted, for over twenty years, to have a rich and complex phase space of colloidal crystals. However, experiments have consistently suggested that such crystals are kinetically inaccessible, as small amounts of polydispersity poison crystal formation. Here, we show a result of small-angle X-ray scattering experiment of highly polydisperse (yet monomodal) colloidal dispersions in a range of sizes (average size from 8 to 50 nm), with soft, charge-mediated interactions. These dispersions were dialysed and compressed by aqueous solutions of poly(ethylene glycol) to reach 15% to 30% of volume fraction, and crystallize. Their phase diagrams, structure factors and crystal peaks were analysed by the x-ray scattering patterns. We found coexistences of complex crystal structures (two BCC structures and Laves AB2) for the small particle size, and BCC and FCC crystals for the larger particle size. These results show a fractionation among the particles. We further show how this is possible through numerical simulations, which explain how the fractionation occurs and how the particles distribute among the different coexisting phases.

CPP 6.3 Mon 10:15 H51

Free energies, liquid and crystal phases of the Asakura–Oosawa model: a density functional theory study — •Mostafa Mortazavifar and Martin Oettel — Institut für Angewandte Physik, Uni Tübingen, Tübingen, Germany

The Asakura–Oosawa(AO) model is a well known model for studying colloid–polymer mixtures in which the depletion interaction between colloidal particles results in a phase diagram similar to molecular liquids. More importantly, it is a generic model system for short range attractive colloidal particles. We have studied the model by means of density functional theory (DFT) by applying a linearization of a two–component fundamental measure hard sphere tensor functional with respect to the second (polymer) component. The linearized functional gives a unified description of gas, liquid, and crystal phases. We have calculated the free energies and phase diagrams for a variety of colloid–polymer size ratios. The results are in good agreement with available simulations. For small size ratios, the model can be mapped exactly to a one–component system with a short–range attractive potential between the colloids. Standard mean field approximations fail in describing the liquid and crystal phases; here our functional offers novel insights how to construct generically density functional descriptions of interparticle attractions.

CPP 6.4 Mon 10:30 H51

Crystallization of sheared nearly hard-spheres — •david richard and thomas speck — Staudingerweg 9, 55128 Mainz

Understanding crystallization pathways and kinetics is a long standing challenge in condensed matter science. Additionally, the effect of impurities and external fields is also a matter of debate. In this study, we look at the effect of a simple linear shear flow on the crystallization of nearly hard-spheres [1]. By varying the density from low to high supersaturation, we find a crossover from shear-suppressed crystallization to an enhanced crystallization kinetics. We attribute this crossover under shear to the vanishing nucleation barrier in the quiescent system, at which nucleation is changing from an activated to a diffusive limited process.

[1] Richard, David, and Thomas Speck. 'The Role of Shear in Crystallization Kinetics: From Suppression to Enhancement.' Scientific Reports 5 (2015).

CPP 6.5 Mon 10:45 H51

On the influence of the softness of the potential on the phase diagrams of core-shell micelles - a simulation study — •Heiko G. Schoberth, Heike Emmerich, and Thomas Gruhn — Lehrstuhl Material- und Prozesssimulation, Universität Bayreuth, D-95440 Bayreuth

Quasicrystals are of continuous interest due to their fascinating fundamental properties and their promising applications as advanced photonic materials in a range of optical devices. In the last years colloidal quasicrystals have been found in solutions with spherical polymer core-shell micelles. With these colloids and their intriguing possibility to self-assemble in a broad range of nanoscale and microscale quasicrystalline structures, the demand arises of understanding the complex formation mechanism and the thermodynamic stability of these structures. Especially, it is important to find a direct relation between the stability of the structures and the main parameters of the micelle-micelle interaction. We perform coarse-grained molecular dynamics simulation to investigate the dependence of the phase diagram on the softness of the interaction potential. The core-core interaction is modelled by infinite repulsion, whereas the shell-shell interaction is varied from a stiff to a very soft potential. Varying the core to shell radius and packing fraction we study systematically the change in the phase diagram finding domains with 10-,12-,18-,24-fold quasicrystalline symmetries. With increasing smoothness of the potential the phase diagram changes qualitatively and the geometry of the phase boundaries gets more regular.

CPP 6.6 Mon 11:00 H51

Estimation of crystal nucleation barriers for colloidal crystals from computer simulations — •Peter Koss[1,2], Antonia Statt[1], 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

A fluid in equilibrium in a finite volume, with a density exceeding the onset of freezing, may exhibit phase coexistence of a crystal nucleus surrounded by liquid. In classical nucleation theory, the barrier of homogeneous nucleation is given by two contributions, the energy gain of creating a droplet and the energy loss due to surface tension of the newly created interface. Using a computational method suitable for the estimation of the chemical potential of dense fluids we obtain the excess free energy due to the surface of the crystalline nucleus. Our novel 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 report that the nucleation barrier for a soft version of the effective Asakura-Oosawa model[1] is compatible with a spherical shape, and consistent with classical nucleation theory [2].

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

5771 (1999).

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

CPP 6.7 Mon 11:15 H51

Crystal nucleation in metastable hard sphere fluids by confocal microscopy — Achim Lederer[1] and •Hans Joachim Schöpe[2] — [1]Retsch Technology GmbH, Retsch-Allee 1-5, 42781 Haan, Germany — [2]Eberhards Karls Universität Tübingen, Auf der Morgenstelle 10, 72026 Tübingen, Germany

Crystal nucleation in colloidal hard spheres is a longstanding research topic. Light scattering and confocal microscopy as well as simulations had been carried out to characterize the nucleation process and to get a microscopic picture. In these studies results both differ and agree with each other. It is still unclear whether the large disagreement in the nucleation rate densities between the light scattering experiments and simulations are of physical nature or result from differing data analyses. Furthermore, the temporal evolution of the microscopic structure has not yet been characterized sufficiently. Using laser-scanning confocal microscopy we study crystal nucleation in colloidal hard spheres. The used system has been characterized with extreme care to allow for meaningful comparison with other experiments and simulations. Observing a large sample volume we can analyze the nucleation process with high accuracy. This allows us to obtain meaningful data of the nucleation rate density, critical nucleus size and nucleation barrier. Furthermore, we determine the time-dependent interfacial tension through how the cluster size distribution evolves. Analyzing the nucleation process on a microscopic scale, we confirm the scenario of precursor-mediated crystal nucleation. In addition we show in great detail the structure evolution from precursor to crystal.

15 min. break

Invited Talk CPP 6.8 Mon 11:45 H51

Percolation in colloidal model systems — •Tanja Schilling[1], Hugues Meyer[1], Mohit Dixit[1], Mark Miller[2], and Paul van der Schoot[3] — [1]Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg — [2]Department of Chemistry, Durham University, United Kingdom — [3]Theory of Polymers and Soft Matter, Technische Universiteit Eindhoven, 5600 MB Eindhoven, The Netherlands

Connectivity percolation is the transition in which isolated clusters of solid particles in a fluid become connected in some sense to form a system-spanning network. This network has a significant effect on the transport properties of the material on a macroscopic scale. If, for example, an electrically insulating polymer is mixed with conductive fibres such as carbon nanotubes, the conductivity of the composite increases by ten or more orders of magnitude near the percolation transition of the filler material.

We discuss percolation in suspensions of fibres and of platelets. Our study covers the entire range of aspect ratios from spheres to extremely slender rods and infinitely thin disks. The percolation threshold for rod-like particles of aspect ratios below 1000 deviates significantly from the inverse aspect ratio scaling prediction, thought to be valid in the limit of infinitely slender rods and often used as a rule of thumb for fibres in composite materials. We also show the effects of polydispersity on the percolation transition. The main result is that the percolation threshold shows universal behaviour, i.e. it depends only on certain cumulants of the size distribution.

CPP 6.9 Mon 12:15 H51

Towards flexible and dynamic self-assembly from colloids with magnetic anisotropy — •Gabi Steinbach[1,5], Dennis Nissen[2], Manfred Albrecht[2], Ekaterina V. Novak[3], Pedro Sánchez[4], Sofia Kantorovich[3,4], Sibylle Gemming[1,5], and Artur Erbe[5] — [1]Technische Universität Chemnitz, 09107 Chemnitz, Germany. — [2]University of Augsburg, 86159 Augsburg, Germany. — [3]Ural Federal University, 620000, Ekaterinburg, Russia. — [4]University of Vienna, 1090 Vienna, Austria. — [5]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany.

Magnetic colloidal particles are a suitable model system for the study of self-assembly and dynamic processes on the microscale. Here, we illustrate the potential of directed, but flexible bonds for tailored structure formation. As an example, we present a system of colloidal microspheres that have an off-centered net magnetic moment pointing perpendicular to the particle surface. They are an experimental realization of the theoretical model of spheres with radially shifted point dipole (sd-particles). Experimentally we observed the formation of branched structures as result of two coexisting self-assembly patterns, which is untypical for homogeneous systems. We show that the bistability can be explained by an extended model of sd-particles. This framework takes the broad magnetization distribution in the experimental particles into account. We will further show that the interacting particles exhibit interesting non-equilibrium dynamics when exposed to time-dependent fields, leading to reversible structural reconfigurations.

CPP 6.10 Mon 12:30 H51

Enhanced magneto-optical response in dispersions of anisometric pigment particles — •Kathrin May, Alexey Eremin, and Ralf Stannarius — Institute of Experimental Physics, Otto von Guericke University Magdeburg, Universitätsplatz 2, 39016 Magdeburg, Germany

Colloidal suspensions of anisometric particles show a variety of unique properties depending on particle concentration and external electric fields, such as the formation of ordered phases, phase separation, electro-optical effects, and non-linear rheology. Electro- and magneto-optical properties of colloids are of particular interest because of the possible applications in electrophoretic ink displays and other technologies. We demonstrate a binary colloidal system with an unusually strong magneto-optical response which is comparable with that of thermotropic liquid crystals. This system is based on a binary mixture of elongated non-magnetic pigment particles and a small volume fraction < 0.1 v/% of spherical magnetic nanoparticles. The birefringence is caused by a partial alignment of the pigment particles, controlled by anisometric agglomerates of the magnetic particles that form in a magnetic field. This effect is discussed in the frame of the Onsager-Lekkerkerker theory of sterical alignment transfer in binary mixtures of colloidal particles.

The authors acknowledge the support by DFG (SPP 1681).

CPP 6.11 Mon 12:45 H51

The initial magnetic susceptibility of cube-like magnetic colloids in dilute suspensions — •Joe Donaldson[1] and Sofia Kantorovich[1,2] — [1]Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria — [2]Ural Federal University, Lenin av. 51, 620083, Ekaterinburg, Russia

Magnetic nano/micro-particles are currently applied in many diverse research and industrial disciplines. These particles exhibit a number of interesting properties that can be utilised, leading to a number of established and developing applications. Most notably: magnetic drug targeting; magnetic hyperthermia cancer treatment; and ferrofluids. In each of these applications, a crucial piece of information is required; namely, some sort of insight into the magnetic behaviour of these particles. Ideally, one would like some indication of this a priori. As such, we present here theoretical and simulation studies on permanently magnetised particles that are actually cube-like in shape [1]. We have investigated the differences in magnetic behaviour arising from this additional directional interaction, focussing on the initial magnetic susceptibility of low-density suspensions.

[1] J. G. Donaldson and S. S. Kantorovich, Nanoscale, 2015, 7, 3217

CPP 7: Hybrid and Perovskite Photovoltaics I (joint session CPP/DF/DS/HL, organized by CPP)

Time: Monday 15:00–17:30 Location: H38

CPP 7.1 Mon 15:00 H38

Effect of phase transition on photoluminescence polarization of single perovskite nano-objects — •Daniela Täuber[1], Alexander Dobrovolsky[1], Rafael Camacho[1,2], and Ivan Scheblykin[1] — [1]Chemical Physics, Lund University, Lund, Sweden — [2]Department of Chemistry, University of Leuven, Leuven, Belgium

We use 2D polarization resolved microscopy to study the polarization of single $CH_3NH_3PbI_3$ perovskite nano-objects in excitation and emission at 295, 152 and 77 K. Depending on size and shape, polarization of up to 70% was observed at 77 K in emission, while it is in general smaller in excitation, and it decreases with increasing temperature. For wire-shaped objects the polarization is along the long axis, which points to contributions from antenna effects and crystal growth direction in combination with asymmetric crystal structures. The difference seen in excitation and emission may be caused by the band structure and the excitation wavelength at 448 nm.

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

CPP 7.2 Mon 15:15 H38

Energy Levels at Perovskite/Electron Transport Layer Interfaces — •Fengshuo Zu[1], Johannes Frisch[1], Liangsheng Liao[2], and Norbert Koch[1] — [1]Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 6, 12489 Berlin, Germany — [2]FUNSOM,Soochow University, Jiangsu 215123, China

organometal halide perovskites attract substantial attention for high-efficiency thin film solar cells. Numerous studies are focused on film processing and device configuration variation in order to further improve device efficiency, but the fundamental physics in particular regarding interfacial energy level alignment with charge transport materials (e.g., fullerene derivatives) are yet poorly understood. It is generally believed that perovskites form type-II p-n junctions with C60 or PCBM, which would favor the charge separation process at the interface. To substantiate this proposition, we performed TRPL and UPS measurements to investigate the interface energy levels and the charge separation process at perovskite/fullerene junctions. However, contrary to the common believe, our measurements show that both junctions exhibit n-n type-I level alignment. TRPL results show no different decay channels with or without fullerene layers, which indicates the perovskite/fullerene interface does not provide a driving force for charge separation. Nonetheless, our solar cells with PCBM junctions show reasonable performance, with a power conversion efficiency of 9.30%. In constrast, the perovskite/C60 solar cells show much lower efficiency, which we attribute to upward band bending within perovskite when in contact with C60.

CPP 7.3 Mon 15:30 H38

The influence of hole transporting materials on the charge transport in stacked perovskite-based systems — •Kathrin Bader[1,2], Michiel Petrus[1,2], Thomas Bein[1,2], Pablo Docampo[1,2], Matthias Handloser[1,2], and Achim Hartschuh[1,2] — [1]Department of Chemistry and CeNS, LMU Munich — [2]Nanosystems Initiative Munich (NIM)

Hybrid metal halide perovskites have become a focal point of the photovoltaic community as promising candidates for next-generation solar cells. Extremely fast progress in this field has taken efficiencies to over 20 % [1] and lead to the development of a large variety of material compositions, preparation techniques and device structures [2]. Although the fabrication of the perovskite absorber itself is comparably cheap, latest device architectures incorporate the expensive hole transporting material (HTM) spiro-OMeTAD. To reduce the overall production costs for perovskite-based devices alternative organic HTMs have been developed [3]. Here we use a contact-less technique based on time-resolved laser scanning confocal microscopy [4] to visualize the influence of different HTMs on $\mathrm{CH_3NH_3PbI_3}$ thin films. We investigate charge carrier transport properties and photoluminescence lifetimes of individual HTM layers as well as stacked perovskite/HTM systems and identify potential candidates to replace the expensive spiro-OMeTAD in the device structure. [1] Green, M. A. et al., Prog. Photovolt: Res. Appl. 2015, 23, 805-812. [2] Green, M. A. et al., Nature Photon. 2014, 8, 506-514. [3] Petrus, M. L. et al., J. Mater. Chem. A 2015, 3, 12159-12162. [4] Bader, K. et al., ACS Photonics 2015, under review.

CPP 7.4 Mon 15:45 H38

Substrate-dependent electronic structure and film formation of MAPbI3 perovskites — •Selina Olthof and Klaus Meerholz — University of Cologne, Institute for Physical Chemistry, Luxemburger Straße 116, 50939 Köln, Germany

Hybrid organic / inorganic perovskite materials have attracted significant attention in the past years. However, little is known so far about the electronic structure and, more importantly, the energetic alignment at interfaces. Here, we present the investigation of the interface formation between the perovskite MAPbI3 and various substrate materials. The perovskite films are incrementally evaporated in situ while the electronic structure is evaluated using photoelectron spectroscopy (PES). The results show a deviation from the commonly assumed flat band condition, and that dipole formation and band bending dominate the interfaces. More importantly, we find a deviation from the expected perovskite stoichiometry at the interface due to a wide variety of chemical interaction taking place, which are highly dependent on the nature of the substrate material. On metal oxides the perovskite film formation is hindered and it takes up to 30 nm for the density of states of perovskite to emerge in the PES measurements. Therefore, the nature of the substrate not only changes the energetic alignment of the perovskite, but can hinder film formation and introduce gap states as well.

CPP 7.5 Mon 16:00 H38

In-Situ Investigation of Optoelectronic Properties during One-Step Synthesis of $\mathbf{MAPbI_{3-x}Cl_x}$ Perovskite — •Klara Suchan, Justus Just, Martin Kärgell, Dan R. Wargulski, Pascal Becker, and Thomas Unold — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Organometal halide perovskites have emerged as promising absorber materials for solid state solar cells since 2012. With the fast improvement in power conversion efficiency to over 20 %, perovskites have high prospects for low-cost, high efficiency solar cell production. $CH_3NH_3PbI_{3-x}Cl_x$ layers are prepared by a one-step solution based process using $PbCl_2$ and MAI precursors dissolved in DMF. Since solution based processes do not need cost intensive vacuum technology and no high-temperature annealing steps, they yield high potential for industrial implementation. However, little is known about the exact mechanisms during synthesis, leading to poor reproducibility. Employing in-situ photoluminescence and reflection imaging as well as spectroscopy we monitor the growth process. The evolution of optoelectronic properties for various temperature profiles and annealing durations is analysed. Additional X-ray diffraction measurements during various stages of the process are used to evaluate structural changes occurring during film formation.

CPP 7.6 Mon 16:15 H38

Reversible Laser induced Amplified Spontaneous Emission from Coexisting Tetragonal and Orthorhombic Phases in Hybrid Lead Halide Perovskites — •Fabian Panzer[1,2,3], Sebastian Baderschneider[2,4], Tanaji Gujar[5], Thomas Unger[1,2], Heinz Bässler[2], Ralf Moos[3], Mukundan Thelakkat[5], Richard Hildner[2,4], and Anna Köhler[1,2] — [1]Experimental Physics II — [2]Bayreuth Institute of Macromolecular Research (BIMF) — [3]Department of Functional Materials — [4]Experimental Physics IV — [5]Applied Functional Polymers, Macromolecular Chemistry I, University of Bayreuth, 95440 Bayreuth, Germany

Organic-inorganic mixed halide perovskites received enormous attention over the last few years due to their outstanding performances when used as absorber material in solar cells or in light emitting devices, while offering the possibility for low cost production, e.g. by solution-processing. Furthermore it is known that most halide perovskite materials can exist in different crystal structures, depending on environmental conditions such as temperature. Here we show that a coexistence of tetragonal and orthorhombic phases within the same crystalline grain can be optically induced into the halide perovskite $\mathrm{CH_3NH_3PbI_3}$ at low temperatures, leading to amplified spontaneous emission simultaneously at two distinct wavelengths. The emission feature associated with the tetragonal phase can be reproducibly written, read-out, and erased at 5 K by choosing appropriate laser fluences or raising the temperature. Finally we show to which extend our findings can be exploited for use as an all optical data storage device.

15 min. break

CPP 7.7 Mon 16:45 H38

Iodine Migration and its Effect on Hysteresis in Perovskite Solar Cells — Cheng Li[1], Steffen Tscheuscher[2], Fabian Paulus[3], Paul Hopkinson[3], Johannes Kiessling[1], Anna Köhler[2], Yana Vaynzof[3], and •Sven Hüttner[1] — [1]Organic and Hybrid Electronics, Makromol. Chemie I, Universität Bayreuth — [2]Experimentalphysik II, Universität Bayreuth — [3]Centre for Advanced Materials, Universität Heidelberg

Solution-processed organic-inorganic hybrid perovskite solar cells (e.g. $CH_3NH_3PbI_3-xCl_x$) currently exhibit promising performances. However, the origin of the observed hysteresis in the current-voltage (J-V) curves, i.e. the sweeping-history-dependent electrical current, is still not sufficiently understood. To investigate its origin we employ electroabsorption (EA) spectroscopy to explore the built-in potential in working photovoltaic devices. Furthermore, we study the temperature dependent dynamic processes in perovskite solar cells by characterizing their current-voltage behavior at different temperatures. The electrical current relaxation process during temperature dependent J-V measurements provides the evidence of the migration of ions. In order to investigate the nature of these ions, we further present X-ray photoemission spectroscopy (XPS) experiments which shows the elemental redistribution after applying an electrical bias. The results give a concise picture that mainly iodide ions can be driven by an external electrical field and then accumulate at the respective perovskite/electrode interfaces. The migration and accumulation of iodide ions create a modulation of the respective interfacial barriers which is the origin of the hysteresis.

CPP 7.8 Mon 17:00 H38

The Importance of Hydrogen Defect Migration in Organic-Inorganic Perovskites — •David A. Egger[1], Leeor Kronik[1], and Andrew M. Rappe[2] — [1]Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel — [2]The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323, USA

Solar cells based on organic-inorganic perovskites have been proven to be remarkably efficient in recent years. However, they exhibit hysteresis in the current-voltage curves, and their stability properties, especially in the presence of water, are problematic. Both issues are possibly related to ionic diffusion phenomena occurring in the hybrid perovskite material. Using first-principles calculations based on density functional theory, we study the properties of an important defect in hybrid perovskites - interstitial hydrogen.[1] We show that differently charged defects occupy different sites in the hybrid perovskite crystal, which allows for an ionization-enhanced defect migration following the Bourgoin-Corbett mechanism. Our analysis further highlights the structural flexibility of organic-inorganic perovskites, where successive displacements of iodide combined with hydrogen bonding enables proton diffusion with low migration barriers. These findings indicate that hydrogen species can be highly mobile in hybrid perovskite solar cells and thus relevant for their performance.
[1] Angew. Chem. Int. Ed. 54, 12437 (2015)

CPP 7.9 Mon 17:15 H38

Humidity-induced hydration of methylammonium lead iodide perovskite: Understanding and prevention — •Yinghong Hu[1], Pablo Docampo[1], Aurélien Leguy[2], and Piers Barnes[2] — [1]Department of Chemistry, Ludwig-Maximilians-Universität, 81377 München, Germany — [2]Physics Department, Imperial College, London, SW7 2AZ, United Kingdom

The long-term stability of hybrid metal halide perovskite solar cells is of paramount importance for the future of this emerging technology. In particular, solar cells composed of methylammonium lead iodide (MAPI) are notorious for their sensitivity to moisture. Here, we elucidate the humidity-induced degradation mechanisms occurring within the perovskite material and report on the development of a novel interlayer which improves the moisture stability of perovskite solar cells. Our results show that MAPI undergoes a stepwise transformation into two species of hydrated MAPI crystal phases upon exposure to moist air at room temperature. However, we show that this hydration process can be reversed when the material is subsequently dried in nitrogen. In contrast to water vapor, the presence of liquid water directly leads to the irreversible decomposition of MAPI to form lead iodide. Our developed functional moisture barrier significantly enhances the stability of the perovskite solar cells towards cycles of hydration and dehydration. We believe that our results open new possibilities for the design of moisture resistant, highly efficient perovskite solar cells.

CPP 8: Hydrogels and Microgels

Time: Monday 15:00–17:45 Location: H40

Invited Talk CPP 8.1 Mon 15:00 H40

The role of nonlinearities and kinetics at phase transitions in stimuli-responsive polymer solutions and hydrogels — •Martine Philipp, Winfried Petry, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Soft condensed matter often self-assembles in a very rich and complex morphology. Typical examples include block copolymer, surfactant, and colloidal systems. Understanding self-assembly involves understanding of phase transitions, particularly of demixing phase transitions, including their kinetics. Crucial parameters on molecular scales are changes in intermolecular interactions, in conformations, and transport processes. During phase transformations, states of less stability are generally passed through. This potentially provokes mechanical instabilities, manifesting by softening. As the linear elastic moduli are small for intrinsically soft materials and as they might even further decrease by transition-induced softening, one can speculate whether elastic nonlinearities can dominate the elastic instability, and hence self-assembly. Analogies known from solid state physics are acoustic soft modes, which govern structural phase transitions in ferroelastic crystals.

In this talk, the impact of elastic, thermo-mechanical and thermo-optical nonlinearities on the order parameter susceptibilities will be discussed for so-called volume phase transitions within stimuli-responsive polymer solutions and hydrogels. First insights into a molecular-mechanistic understanding are presented.

CPP 8.2 Mon 15:30 H40

Impact of the cononsolvency effect on the temperature response of PNIPAM microgels in water/ethanol-mixtures — •Sebastian Backes and Regine von Klitzing — Technische Universität Berlin, Stranski-Laboratorium für Physikalische und Theoretische Chemie, Berlin, Germany

Microgels made of N-isopropylacrylamide (NIPAM) are of great interest because of their pronounced temperature response in solution. They possess a volume phase transition temperature (VPTT) below which they are swollen. When the VPPT is exceeded, the gels expel the solvent and shrink. Both pure water and several pure organic solvents like ethanol are good solvents for PNIPAM. In mixtures of water and ethanol however the solubility is significantly decreased, with the microgels showing a minimum volume at a certain mixing ratio of ca. 20% (cononsolvency effect).

After adsorption on a solid substrate the mixing ratio for the minimum value increases from 20% to about 40-50%. Therefore the volume of microgels has been examined both in bulk using dynamic light scattering and on silica wafers using atomic force microscopy for several water/ethanol mixtures and a temperature range from 10 to 50°C.

The volume phase transition temperature has been shown to decrease from 32°C in pure water to values below the measuring range (i.e. <10°C) for intermediate mixing ratios. At higher ethanol content the VPTT reappears in a broadened form rather than a sharp transition.

CPP 8.3 Mon 15:45 H40

Cononsolvency in thermoresponsive micellar solutions: Pathway of aggregate formation — Konstantinos Kyriakos[1], Anatoly V. Berezkin[1], Martine Philipp[1], Alessio Zaccone[1], Isabelle Grillo[2], Anna Miasnikova[3], André Laschewsky[3,4], Peter Müller-Buschbaum[1], and •Christine M. Papadakis[1] — [1]Technische Universität München, Physik-Department, Garching, Germany — [2]Institut Laue-Langevin, Grenoble, France — [3]Universität Potsdam, Institut für Chemie, Germany — [4]Fraunhofer Institut für Angewandte Polymerforschung, Potsdam-Golm, Germany

The switching kinetics of thermoresponsive polymers are of importance for many applications. In mixtures of water and a cosolvent, the cloud point may be reduced, which offers additional possibilities for switching.

We have investigated the switching kinetics of thermoresponsive poly(N-isopropylacrylamide) (PNIPAM) homopolymers and of micelle forming PS-*b*-PNIPAM (PS stands for polystyrene) diblock copolymers in two ways: (i) by addition of the cosolvent methanol to aqueous solutions of the two polymers [1] and (ii) by rapidly heating a PS-*b*-PNIPAM solution through the cloud point [2]. The aggregate growth was followed by time-resolved small-angle neutron scattering. The process is very different for PNIPAM and for PS-*b*-PNIPAM and depends sensitively on the pathway. We have developed theoretical models to relate the growth rate to the interaction between the collapsed micelles.

1.K. Kyriakos et al., *Macromolecules* 2014, **47**, 6867

2.K. Kyriakos et al., *Macromol. Rapid Commun.*, in press.

CPP 8.4 Mon 16:00 H40

Thermal traps trigger sol-gel phase transitions of DNA with single base sequence selectivity — •Christof B. Mast, Matthias Morasch, Emil Agerschou, Jonathan Liu, and Dieter Braun — Systems Biophysics, Physics Department, Center for Nanoscience, LMU Munich, Germany

Sol-gel phase transitions of DNA normally require long strands, high concentrations and multivalent ions for condensation. We demonstrate that a thermal gradient across a water-filled chamber creates DNA hydrogels from dilute, nanomolar concentrations of short, 36 nts DNA strands without condensation agents. The thermal gradient leads to fluid convection and thermophoresis, which in combination accumulate long biomolecules over short ones. The DNA is composed out of three self-complementary sequences which elongate by hybridization once millimolar concentrations are achieved. At nanomolar concentration, the DNA is an unbound single molecule. Inside the thermal gradient, the molecules accumulate and the self-complementary DNA connect cooperatively to longer and subsequently even better accumulating strands, ultimately leading to the formation of a DNA hydrogel. This localized phase transition is highly sequence selective: self-elongating DNA with a single base pair change per binding site separates from the unchanged DNA upon gelation which leads to the formation of two distinct, sequence pure gels. One single point-mutation at a single binding site can prevent the formation of the hydrogel. The mechanism implements a prebiotic machine that selects and stores oligonucleotides with very similar sequences starting from nanomolar concentration.

15 min. break

CPP 8.5 Mon 16:30 H40

Linear thermoresponsive surface coatings based on acrylamide microgels — Oliver Wrede, Johannes Bookhold, Marian Cors, and •Thomas Hellweg — Bielefeld University, Germany

Polymer coatings are used in a wide range of applications, such as anti fouling, enhancement of wetting abilities or corrosion protection. Combined with stimuli-responsive materials like acrylamide based microgels even more implemantations are possible. In these microgels, an external stimulus like temperature, pH or ionic strength leads to a response in the particle size. To implement the particles into systems like sensors or nanoactuators, a well known and precise control of the stimuli response must be obtained. Therefore, we investigated complex microgel architectures obtained by a two-step synthesis protocol. These exhibit a reversible linear size response upon a temperature stimulus. Even if the particles are deposited onto surfaces, this linear dependency of the size on the temperature is still preserved. The properties of the particles and therefore those of the resulting surfaces can be modified by selecting specific conditions during the synthesis (surfactant concentration, cross linker content, etc.). Creating tailor-made surfaces that fullfill the demands of future applications is therefore possible.

CPP 8.6 Mon 16:45 H40

Swelling kinetics of N-*n*-propylacrylamide based microgels upon periodic pressure jumps investigated by time-resolved SANS — •Oliver Wrede[1], Yvonne Pütz[2], Stefan Lülsdorf[3], Diana Zauser[3], Yvonne Hertle[1], Ralf Schweins[4], Thomas Sottmann[3], and Thomas Hellweg[1] — [1]Bielefeld University, Germany — [2]University of Cologne, Germany — [3]University of Stuttgart, Germany — [4]Institut Laue-Langevin, France

Temperature responsive microgels are particles in the size range between 100 nm and 1 μm, that undergo a reversible microphase seperation at a certain temperature. Structure, size and phase transition properties can be controlled by the synthetis conditions. This makes them outstanding candidates for various applications, such as drug delivery, catalytic particle carriers or nanoactuators. A precise understanding of the underlying processes is necessary to allow to tune the network properties. Therefore, we investigated the swelling and deswelling kinetics of N-*n*-propylacrylamide based microgels upon periodic pressure jumps across the phase transition with different cross-linker contents by time-resolved SANS. Preceding DLS measurements showed, that the phase transition shifts towards higher temperatures with increasing pressure, i.e. a swelling of the particles is induced upon compression. Our findings show, that the time scale of the kinetics changes with cross-linker content by more than one order of magnitude, which confirmes the important role of the network morphology. Besides the influence of the cross linker, the kinetics of the swelling is considerably faster than the deswelling process.

CPP 8.7 Mon 17:00 H40

Superresolved fluorescence and electron microscopy to visualize the core-shell structure of microgels — •Dominik Wöll[1], Arjan Gelissen[1], Alex Oppermann[1], Tobias Caumanns[2], Pascal Hebbeker[1], Rahul Tiwari[3], Joachim Mayer[2], Walter Richtering[1], and Andreas Walther[3] — [1]Institute of Physical Chemistry, RWTH Aachen University, Landoltweg 2, 52056 Aachen, Germany. — [2]GFE Central Facility for Electron Microscopy, RWTH Aachen University, Mies-van-der-Rohe-Straße 59, 52074 Aachen, Germany. — [3]DWI - Leibniz-Institute for Interactive Materials, Forckenbeckstr. 50, 52074 Aachen, Germany

Microgels are an interesting class of soft matter materials with properties depending on their internal structure. Electron and superresolved fluorescence microscopy will be presented as methods to open up the possibility to visualize the core-shell structure of single microgels. In both cases, appropriate labelling conditions had to be chosen to gain sufficient contrast. As the approaches used so far cannot distinguish between different axial (z-)position, the obtained images consist of 2D projections of the 3D positions of labels. From these projections, we developed a method to calculate the 3D radial distribution function using appropriate core-shell models established in microgel research.

CPP 8.8 Mon 17:15 H40

CP-AFM Study on elastically switchable core-shell microgel particles with constant adhesion properties — •Maximilian Seuss[1], Willi Schmolke[2], Sebastian Seiffert[2], and Andreas Fery[1] — [1]Leibniz Institute of Polymer Research Dresden, Dresden, Germany — [2]Institute of Chemistry and Biochemistry, FU Berlin, Berlin, Germany

We present a novel class of thermo-responsive core-shell microgel particles. They allow to change their mechanical properties while their adhesive properties remain unaffected. The switching is introduced by a thermo-responsive hydrogel core exhibiting a volume phase transition, e.g. poly(N-isopropylacrylamide). Exceeding its lower critical solution temperature, the microgel deswells, densifies, and therefore becomes stiffer. Usually, this process is accompanied by a change in surface chemistry since the microgel switches from hydrophilic to hydrophobic.[1] These effects can be decoupled from each other by encapsulating the microgel in a thermally non-responsive polyacrylamide shell in a droplet-based microfluidics approach.[2] Using colloidal probe AFM, we validated the constant adhesion properties of such core-shell particles between 28 and 40 °C. Further, we have proven that the elastic changes of the core material are preserved attenuatedly in the corresponding core-shell microgel particles.

[1] S. Schmidt, Adv. Funct. Mater. 2010, 20, 3235

[2] S. Seiffert, J. Am. Chem. Soc. 2010, 132, 168

CPP 8.9 Mon 17:30 H40

Microgel ultrafiltration — •Rafael Roa[1], Jonas Riest[2], and Gerhard Naegele[2] — [1]Helmholtz-Zentrum Berlin, Institute for Soft Matter and Functional Materials, Berlin, Germany —

[2]Forschungszentrum Juelich, Institute of Complex Systems (ICS-3), Juelich, Germany

Membrane ultrafiltration (UF) is a pressure driven process allowing for the separation and enrichment of protein solutions and dispersions of nanosized microgel particles. The permeate flux and the near-membrane concentration-polarization (CP) layer in this process is determined by advective-diffusive dispersion transport and the interplay of applied and osmotic transmembrane pressure contributions. The UF performance is thus strongly dependent on the membrane properties, the hydrodynamic structure of the Brownian particles, their direct and hydrodynamic interactions, and the boundary conditions. We present a macroscopic description of cross-flow UF of microgels. We analyze the CP layer properties and the permeate flux at different operating conditions. Our results show that the proper specification of the concentration-dependent transport coefficients is important for reliable filtration process predictions. We also show that the solvent permeability of microgels is an essential ingredient to the UF modeling. The particle permeability lowers the particle concentration at the membrane surface, thus increasing the permeate flux.

CPP 9: Nanoparticles, Nanocrystals and Composites II

Time: Monday 15:00–16:30 Location: H41

CPP 9.1 Mon 15:00 H41

Tailoring metal nanoparticle layers at the polymer-metal interface — •Stephan V. Roth[1], Matthias Schwartzkopf[1], Oleksandr Polonskyi[2], Alexander Hinz[2], Thomas Strunskus[2], Franziska Löhrer[3], Volker Körstgens[3], Franz Faupel[2], and Peter Müller-Buschbaum[3] — [1]DESY, Notkestr. 85, 22607 Hamburg — [2]CAU zu Kiel, Kaiserstr.2, 24143 Kiel — [3]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Organic photovoltaic cells, flexible electronics and sensors crucially rely on nanostructuring of thin films at the polymer-metal interface [1]. Here, vacuum deposition of metal layers offers a versatile route for fabricating tailored metal arrays, ranging from isolated nanoparticles to full scale electrical contacts. The interaction of the metal atoms with the underlying polymer template (e.g. wetting) as well as the relevant deposition conditions (e.g. deposition rate and bias-voltage) play a crucial role and influence both the metal layer growth and the development of the near-surface interface in the polymer-metal nanocomposite. We observe in real-time the industrial relevant aluminium layer installation in the different growth modes from nucleation to percolation during sputter deposition on polymer template. Combining in-situ x-ray scattering and ellipsometry, we thus correlate the structural and morphological characteristics of the polymer-metal interface with its optical properties. [1] Roth et al., ACS. Appl. Mater. Interfaces 7, 12470 (2015), & J. Appl. Cryst. 48, 1827 (2015)

CPP 9.2 Mon 15:15 H41

In-situ investigation of aluminum thin film growth on a nanostructured diblock copolymer substrate — •Björn Beyersdorff[1], Matthias Schwartzkopf[1], Deniza Chekrygina[2], Valentia Cantelli[3], Ezzeldin Metwalli[4], Senlin Xia[4], Carsten Baehtz[1,3], Peter Müller-Buschbaum[4], and Stephan V. Roth[1] — [1]DESY, Hamburg — [2]Universität Hamburg — [3]Helmholtz-Zentrum Dresden-Rossendorf — [4]Technische Universität München

Targeted installation of nanostructured metal films for application devices is of utmost 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 from the deep UV to the infrared region [1].

When depositing metal on a nanostructured diblock copolymer substrate, a different adatom mobility on the two polymer blocks often leads to selective wetting and thus to nanostructure formation [2,3]. We investigated the sputter deposition of Al on a PS-b-PMMA diblock copolymer thin film by means of grazing incidence small-angle X-ray scattering (GISAXS). The resulting GISAXS pattern yield information on the different growth regimes during nanostructural evolution as well as on the modification of the diblock copolymer substrate due to the Aluminum deposition. [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 9.3 Mon 15:30 H41

When do clusters start to behave like a solids: A density-functional theory study of noble gas clusters — •Lydia Nemec[2], Benjamin Johnson[1], Oliver T. Hofmann[3], Alexander M. Bradshaw[5], and Patrick Rinke[4] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Technische Universität München — [3]Technische Universität Graz, Austria — [4]Aalto University, Helsinki, Finland — [5]MPG für Plasmaphysik (IPP), Germany

Weakly bonded argon clusters are a popular model system for studying the transition from molecular to bulk behaviour. Angle-resolved photoemission spectra exhibit bulk-like energy dispersion for clusters as small as 200 atoms [1]. To investigate this observation, we performed a density functional theory (DFT) study of Ar and Kr clusters using the all-electron, numeric, atom-centered basis function code FHI-aims. We use semilocal density functionals including van der Waals dispersion terms in the Tkatchenko-Scheffler approach (PBE+vdW). We developed a method to translate cluster states to a k-resolved energy dispersion based on a Fourier transformation of the eigenstates. For low-energy structures taken from the structure database [2], we show that already clusters in the 200 atom size range exhibit a bulk-like atomic structure. We then demonstrate the emergence of a band-like energy dispersion with increasing cluster size. Finally, we discuss the influence of spin-orbit splitting by contrasting Ar with Kr.

[1] Förstel, *et. al*, J. El. Spec. Rel. Ph. 184, 107-112 (2011) [2] Y. Xiang,*et. al*, J. Phys. Chem. A, 108, 3586-3592 (2004)

CPP 9.4 Mon 15:45 H41

Nucleation and Growth Kinetics of Multinary Nanocrystals by Quick Extended X-ray Absorption Fine Structure — •Justus Just[1,2], Oliver Müller[2], Claudia Coughlan[3], Kevin M. Ryan[3], Dirk Lützenkirchen-Hecht[2], Ronald Frahm[2], and Thomas Unold[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Bergische Universität Wuppertal, Gaußstraße 20, 42109 Wuppertal, Germany — [3]Materials and Surface Science Institute and Department of Chemical and Environmental Sciences, University of Limerick, Limerick, Ireland

Early stage nucleation and subsequent growth of multinary nanocrystals (Cu_2ZnSnS_4) are investigated by real time in-situ measurements of the X-ray absorption fine structure at the Cu and Zn K-edges in conjunction with simultaneously measured small angle X-ray scattering and optical transmission. The specially designed hot-injection reaction setup as well as the QEXAFS experimental setup allows to investigate the chemical reaction within timescales of several 10 ms which especially enables the investigation of early reaction stages. We found the monodispersed rod shaped hexagonal nanocrystals to grow within six well distinguishable reaction stages, the kinetics of which are influenced by the choice of ligands and solvents.

CPP 9.5 Mon 16:00 H41

Characterization of active iron cites in Fe-ZSM-5 catalysts using Mössbauer spectroscopy — •Kydala Ganesha Padmalekha[1], Heming Huang[1], Inga Ellmers[2], Roxana Pérez Vélez[3], Angelika Brückner[3], Wolfgang Grünert[2], and Volker Schünemann[1] — [1]Department of Physics, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Lehrstuhl Technische Chemie, Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum, Germany — [3]Leibniz-Institut für Katalyse e. V., 18059 Rostock, Germany

Fe-ZSM-5 catalysts are important in catalytic reduction of NOx by NH3 in vehicle exhausts. The iron centres in the hetergogeneous catalyst can exist in various forms and oxidation states after iron loading and pretreatment and it is non trivial to identify and quantify them. We have investigated isotopically enriched 57Fe-ZSM-5 (Si/Al ~ 14, <= 0.7 wt% Fe), which was prepared via solid-state ion exchange, before and after standard selective catalytic reduction SCR (sSCR) using field dependent Mössbauer spectroscopy. We present deconvolution of the spectra into contributions from the different iron species and their corresponding abundances. We use a five component analysis of the spectra using ferric iron oxide, ultrasmall ferric iron agglomorates a part of which are diamagnetic, paramagnetic ferrous high spin ions and two kinds of paramagnetic ferric high spin ions which were detected using EPR spectroscopy.

CPP 9.6 Mon 16:15 H41

BaTiO3 Modifications for Photochemical Hydrogen Evolution — •yan xiong and frank marlow — Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr, Germany

The perovskite-type material BaTiO3 is a wide-bandgap semiconductor and a prospective material for the photochemical hydrogen evolution via water splitting. In our work, we studied reduction-treatments of BaTiO3 and the effect of Pt as a co-catalyst on BaTiO3 for the hydrogen evolution reaction. We found that the catalytic activity of reduced-BaTiO3 is enhanced by a factor of 1.5 compared to the original material. The rates of hydrogen generation of reduced and bare BaTiO3 are 159 and 100 μmol/h, respectively. The effect of Pt as a co-catalyst on BaTiO3 is non-linear. The photocatalytic activity increases up to 527 μmol/h with the increasing Pt amount up to 1 wt.% and decreases above this amount. In our study reduced BaTiO3 with 1 wt.% Pt has shown the best performance.

CPP 10: Colloids and Complex Fluids III (joint session BP/CPP/DY, organized by CPP)

Time: Monday 15:00–18:00 Location: H42

CPP 10.1 Mon 15:00 H42

Directed assembly of soft colloids through rapid solvent exchange — •Arash Nikoubashman[1], Victoria E. Lee[2], Chris S. Sosa[2], Robert K. Prud'homme[2], Rodney D. Priestley[2], and Athanassios Z. Panagiotopoulos[2] — [1]Institute of Physics, Johannes Gutenberg University of Mainz, Germany — [2]Department of Chemical and Biological Engineering, Princeton University, USA

We studied the directed assembly of soft nanoparticles through rapid micromixing of polymers in solution with a non-solvent. Both experiments and computer simulations were performed to elucidate the underlying physics and to investigate the role of various process parameters. In particular, we discovered that no external stabilizing agents or charged end-groups are required to keep the colloids separated from each other, when water is used as the non-solvent. The size of the nanoparticles can be reliably tuned through the mixing rate and the ratio between polymer solution and non-solvent. Furthermore, we were able to fabricate a wide variety of patchy colloids, such as Janus particles, when polymer blends were used in the feed stream. Our results demonstrate that this mechanism is highly promising for the mass fabrication of uniformly-sized colloidal particles, using a wide variety of polymeric feed materials.

CPP 10.2 Mon 15:15 H42

Directed Assembly of Janus Particles through Flow — •Arash Nikoubashman — Institute of Physics, Johannes Gutenberg University of Mainz, Germany

We investigate the self-assembly of colloidal Janus particles under shear and Poiseuille flow, by employing hybrid molecular dynamics simulations that explicitly take into account hydrodynamic interactions. Under quiescent conditions, the amphiphilic colloids form spherical aggregates with a large size polydispersity. The solvophobic hemispheres are directed towards the core, whereas the solvophilic caps are exposed to the solvent. When sufficiently strong shear is applied, the micelles disaggregate with a consequent decay of the average cluster size. However, we find an intermediate regime where the balance between rearrangement and dissociation favors the growth of the aggregates, where the majority of clusters consist of 13 particles in an icosahedral arrangement. This bias is due to the high geometric symmetry of the icosahedron, which maximizes the internal bonding energy of the aggregate. Our findings demonstrate how self-assembly can be directed towards specific structures via external fields, and open up new applications for Janus particles, ranging from biotechnology to sensor systems.

CPP 10.3 Mon 15:30 H42

Self-organized velocity pulses of dense colloidal suspensions in microchannel flow — •Philipp Kanehl and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany

Colloids in dense suspension exhibit shear-induced migration and size segregation under pressure driven flow [1]. If the density is increased further, the steady flow becomes unstable and regular oscillations in flow velocity emerge [2]. To develop a theoretical understanding of these oscillations, we simulate colloidal particles with frictional contact under pressure-driven flow in two dimensions using the mesoscale simulation technique of multi-particle collision dynamics.

We present a detailed parameter study on how friction generates transient jamming in the colloidal flow. The jammed regions are unjammed by rarefaction pulses travelling upstream similar to the experimental observations. Moreover, we address the role of fluid permeation and channel confinement.

Finally, a linear stability analysis of a newly developed continuum model predicts scaling laws for stability condition, wavenumber, and pulse speed, which agree well with our numerical data.

[1] P. Kanehl and H. Stark, J. Chem. Phys. 142, 214901 (2015).

[2] L. Isa, R. Besseling, A. N. Morozov, and W. C. Poon, Phys. Rev. Lett. 102, 058302 (2009).

CPP 10.4 Mon 15:45 H42

An empirical correction for multiple scattering in integral laser Doppler velocimetry experiments — •Denis Botin[1], Ludmila Marotta Mapa[1,2], Christopher Wittenberg[1], Holger Schweinfurt[1], and Thomas Palberg[1] — [1]Institute of Physics, JGU, D-55099, Mainz, Germany — [2]Federal Univesity of Itajuba, Brazil

Super-heterodyne laser Doppler velocimetry (SHLDV) provides an integral measurement of the velocity distribution in electro-kinetic experiments[1]. This allows simultaneous evaluation of the electro-phoretic and electro-osmotic mobilities of the particles and along the cell wall, respectively [2]. Here, we introduce an extension of the method to the regime of concentrated samples, where multiple scattering affects the signal [3]. Multiple scattering distorts the signal shape, creating an additional hump in the background and prohibiting any meaningful fit. We use an empirical correction scheme for the spectra, in which we fit the multiple scattering contribution and subtract it from the raw data. This leaves the velocity dependent singly scattered contribution unaffected. First applications to measurements of the concentration dependence of the electro-phoretic mobility of charged colloidal spheres are reported.

[1]T. Palberg et al. J. Phys. Chem. 96, 8180 - 8183 (1992)

[2]T.Palberg et al. J. Phys.: Condens. Matter 24, 464109 (2012).

[3]H.C. Van de Hulst., *Multiple Light Scattering: Tables, Formulas, and Applications*, Academic Press, New York., (1980).

CPP 10.5 Mon 16:00 H42

Multiscale modelling of complex (macro-)molecular fluid mixtures — •Christoph Junghans[1], Tiago E. de Oliveira[2,3], Paulo A. Netz[2,3], Debashish Mukherji[2], and Kurt Kremer[2] — [1]CCS Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA — [2]Max-Planck Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz Germany — [3]Universidade Federal do Rio Grande do Sul, Porto Alegre, Brazil

Many biophysical processes in water are determined by the interactions of cosolvents within the hydration shells of dissolved molecules. Computational approaches are mostly limited to the “mid sized" all-atom simulation protocols. While all-atom simulations are suitable in some cases, problems arise when concentration fluctuations are large, thus requiring efficient simulation methods. Therefore, we develop two distinct, yet related, multiscale methods. In one case, we develop a semi-grand canonical MD that heals the particle depletion [1] that uses the AdResS scheme [2], coupled with a metropolis particle exchange criterion. In AdResS, an all-atom region is coupled to a coarse-grained (CG) reservoir, where the particle exchange is performed. In the second protocol, we develop a “parameter free" CG model, which uses cumulative coordination within an iterative procedure [3]. Both methods preserve pair-wise structure of complex fluids and their solvation thermodynamics. We apply these methods to study several cases of (macro)molecular solvation in aqueous mixtures [1,3].

[1] D. Mukherji and K. Kremer, Macromolecules (2013). [2] S. Fritsch, et al. PRL (2012). [3] T. E. de Oliveira, et al. (2016).

CPP 10.6 Mon 16:15 H42

Kinetics of liquid-liquid phase transition in protein solutions exhibiting LCST phase behavior studied by USAXS — •Fajun Zhang[1], Stefano Da Vela[1], Michal Braun[1], Michael Sztucki[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]ESRF, Grenoble, France

We present the results of the early stage kinetics of liquid-liquid phase separation (LLPS) in protein-salt solutions studied by ultra-small angle x-ray scattering (USAXS). The model system of bovine serum albumin (BSA) with YCl_3 [1,2] shows LLPS and a lower critical solution temperature (LCST) phase behavior and can be rationalized using an ion-activated patchy-colloid model [3]. We focus on the phase transition of the dense liquid phases after a T-jump aiming at the arrested or slowed down kinetics. The USAXS curves of sample solutions after a T-jump exhibit a peak that grows in intensity and shifts to lower q values with time. The characteristic length (ξ) obtained from this scattering peak increases with time approximately as $t^{0.3}$. The interface between the dilute and dense phase is quickly established as a Porod region (q^{-4}) is visible within a few seconds. Thus the kinetics of the intermediate stage of phase transition was followed by USAXS. It is interesting to see that ξ(t) is nearly independent on the jump temperatures (below 40 °C). At a higher temperature jump (45 °C), a slowed down kinetics was observed indicating that the gelation line was approached. [1] F. Zhang, et al. Phys. Rev. Lett. 101, 148101 (2008) Proteins 78, 3450 (2010). [2] F. Zhang, et al. Soft Matter 8, 1313 (2012). [3] F. Roosen-Runge, et al. Sci. Rep. 4, 7016 (2014).

15 min. break

CPP 10.7 Mon 16:45 H42

Hydration and hysteresis of triblock copolymers — •Bernhard Schummer, Stefan Gerth, and Randolf Hanke — Universität Würzburg, Lehrstuhl für Röntgenmikroskopie

Ternary polyether are block ABA copolymers consisting of polyethyleneoxide (PEO) (A) and polypropylenoxide (PPO) (B). They change their hydrophilic or hydrophobic balance dramatically with their temperature and their concentration in water. This change causes a micelleisation. In this case P123 will be used as a copolymer and SAXS will be the method of examination. For micelles an appropriate model is the core-shell model where the shell mostly consists of PEO and the core mainly of PPO. In this model the SLD's for core and for shell heavily depend on each other. A new parameter $\kappa = \frac{\rho_c - \rho}{\rho_s - \rho}$ is presented to describe the change of the conformation and hydration of the micelle while including the radii of shell and core. Here ρ_c is the SLD of the core ρ_s the SLD of the shell and ρ the SLD of the solvent. The new parameter indicates that the SLD of the core decreases and thus dehydrates with increasing temperature. For instancethe SLD's of the poloxamer L51 show a similar dependency as P123. The heating and cooling curves of the sample for different small concentrations will be presented and show a hysteresis in the form phase diagram. This can be observed in a diagram where κ is ploted against the temperature. At higher concentrations poloxamers form a liquid crystal. It has already been shown that there is a hysteresis in the cell parameter at high concentrations. This effect can now be attributed to a single component of the system, the form change of the micelle.

CPP 10.8 Mon 17:00 H42

Phase behaviour and interactions in a three components γ-globulin based depletion interaction system — •Stefano Da Vela[1], Fajun Zhang[1], Sarah El-Asfar[1], Christian Exner[1], Michael Sztucki[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]ESRF, Grenoble, France

Aqueous solutions of bovine γ-globulin with polyethylene glycol (PEG) added as non-interacting polymer, provide a tunable protein system for the study of depletion-driven phase behaviour: range and strength of the interaction are adjusted by appropriate choice of PEG molecular weight and concentration. An extensive study of the phase behaviour of the system for different effective attraction strengths reveals a set of conditions for which a Liquid-Liquid Phase Separation (LLPS) phase boundary emerges above the freezing temperature of the solvent. Addition of bovine serum albumin (BSA), results into an effective three components system. BSA, while not inducing depletion interaction on its own, appears to enhance it in presence of PEG, shifting the LLPS boundary to higher temperatures while being preferentially excluded from the resulting protein-dense liquid phase. In order to investigate the effect of BSA on the phase boundaries and on the interaction, phase diagrams as a function of temperature, protein and PEG concentration are presented together with small angle X-ray scattering data. Optical microscopy, turbidimetry and size exclusion chromatography are employed as supplementary techniques. The findings are relevant to the understanding of protein mixtures and their separation.

CPP 10.9 Mon 17:15 H42

Clusters of proteins – are they transient or static? — •Michal Braun[1], Marco Grimaldo[1,2], Felix Roosen-Runge[2], Christian Beck[1], Fajun Zhang[1], Frank Schreiber[1], and Tilo Seydel[2] — [1]Institut für Angewandte Physik, Universität Tübingen, Germany — [2]Institut Laue-Langevin, Grenoble, France

Signatures of protein clusters have been observed for globular proteins such as lysozyme [1], crystallins and bovine serum albumin [2,3]. The nature of these clusters, whether static or transient, however, is still a debated question and depends sensitively on environmental conditions. A better understanding would be key to use protein clusters as precursors for protein crystallization or in drug delivery.

We report cluster formation in solutions of β-lactoglobulin (BLG), as systematically investigated using static and dynamic scattering techniques. From small-angle scattering (SAXS/SANS), we obtain a cluster signature from the missing shift of the correlation peak with concentration and related data fitting. Neutron quasi-elastic backscattering (QENS) evidences the formation of oligomers via the short-time self-diffusion coefficient at nanosecond time scales. Finally, neutron spin-echo spectroscopy (NSE) allows to compare structural information from the structure factor with the dynamical features of collective diffusion on time scales of several tens of nanoseconds, which ultimately allows to determine the nature of the observed protein clusters.

[1] Stradner et al. Nature 432 (2004) 492

[2] Soraruf et al. Soft Matter 10 (2014) 894

[3] Grimaldo et al. J. Phys. Chem. Lett. 6 (2015) 2577

CPP 10.10 Mon 17:30 H42

Self-assembled micelles as drug carriers: Influence of molar mass and chain architecture — •Bart-Jan Niebuur[1], Xiaohan Zhang[1], Natalya Vishnevetskaya[1], Petr Chytil[2], Sergey K. Filippov[2], and Christine M. Papadakis[1] — [1]Technische Universität München, Physik-Department, Garching, Germany — [2]Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Prague, Czech Republic

A promising way to achieve site-specific delivery of anticancer agents is to use the enhanced permeation and retention (EPR) effect of self-assembled polymeric micelles. At this, a low critical micelle concentration (CMC) and particle sizes in the range of 1-100 nm are of importance.

In the present work, we focus on the importance of (i) the overall molar mass and (ii) the chain architecture. We investigate both N-(2-hydroxypropyl) methacrylamide (HPMA) [1] homopolymers with randomly distributed cholesterol side groups and diblock copolymers having a pure HPMA block and an HPMA block with cholesterol. Using fluorescence correlation spectroscopy and small-angle neutron scattering (SANS), the CMC as well as the size and structure of the micelles are determined in phosphate buffer. We find that the CMC decreases with increasing molar mass, but does not depend on chain architecture. The micellar radius is with 4-5 nm in the desired range.

[1] Filippov, S.K. et al., *Biomacromolecules* **13**, 2594 (2012) and **14**, 4061 (2013)

CPP 10.11 Mon 17:45 H42

Modeling Viscoelastic Properties of Complex Fluids — •Julius Schulz, Alexander Schlaich, Roland Netz, and Julian Kappler — Fachbereich Physik, Freie Universiät Berlin, 14195 Berlin

The viscoelastic response of a complex liquid like water differs significantly from more simple models such as a Lennard-Jones fluid or methane. Using all-atom molecular dynamics simulations, we calculate the frequency-dependent viscosity for two liquids: TIP4P/2005 water and a glycerol/water solution. The corresponding elastic spectrum exhibits two peaks and cannot be described by simple viscoelastic models. We discuss the origins of these features and present a novel extension of the Maxwell model for viscoelastic fluids which is capable of reproducing the relevant features of the frequency-dependent viscosity. Extracted shear relaxation times for the glycerol-water mixtures compare well with experiments.

CPP 11: Poster: Hybrid and Perovskite Photovoltaics

Time: Monday 18:15–21:00 Location: Poster B2

CPP 11.1 Mon 18:15 Poster B2

Titania network structures prepared via spray coating for photovoltaic applications — •Bo Su[1], Herbert A. Caller-Guzman[1], Volker Körstgens[1], Christoph J. Schaffer[1], Yuan Yao[1], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]DESY, Notkestr. 85, 22607 Hamburg, Germany

Due to a high surface to volume ratio and their bicontinuous morphology, foam-like network nanostructures are receiving increasing interest in photovoltaic applications. Controlling the pore size is crucial for devices, such as dye-sensitized solar cells (DSSCs) and solid state DSSCs. In this study, 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 the nanostructured titania films. The structure evolution is probed with in situ GISAXS during the spray coating process. The morphology of the sprayed films is characterized with SEM and optical microscopy. The crystalline structure of the titian films is probed with XRD. The optical properties and photoluminescence emission state of the mesoporous titania films are probed by UV vis and photoluminescence, respectively.

CPP 11.2 Mon 18:15 Poster B2

Crystallization behavior of hybrid perovskite films on mesoporous titania templates — •Markus Trunk, Bo Su, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

The tremendous efficiency improvement in organic-inorganic halide perovskite solar cells has attracted very high interest in the last years. Comparing the stability of methylammonium lead halide materials, methylammonium lead bromide ($MAPbBr_3$) is a promising candidate. To increase the device performance with respect to the hysteresis in current-voltage characteristics, we use mesoporous titania films as support layer for the perovskite. We manufactured nanostructured titania films with an additional superstructure in the micrometer-regime. The superstructure was first transferred to a silicon chip via optical lithography. Then, a PDMS stamp was used as a replica of this master stamp and the superstructure was superimposed to the mesoporous titania films via a wet imprinting method. The morphology of wet imprint films is probed by SEM and AFM. The perovskite films are prepared via a one-step method on top of the superstructured mesoporous titania layers. Electronic properties, optical properties and crystalline structure are characterized for these samples.

CPP 11.3 Mon 18:15 Poster B2

Nanostructured zinc oxide films for application in hybrid photovoltaics — •Kun Wang, Lin Song, and Peter Müller-Buschbaum — Physikdepartment E13 Lehrstuhl für Funktionelle Materialien Technische Universität München, James-Franck-Straße 1, München, Germany

Hybrid solar cells, a combination of conventional inorganic photovoltaic systems and organic solar cell technologies, offer outstanding potential due to their minor investment compared to inorganic solar cells and higher stability compared to organic solar cells. In this kind of cells, nanostructured inorganic metal oxides with tunable morphologies are of great importance. Among the many inorganic metal oxides, ZnO has been widely explored due to its outstanding electrical and optical properties and rich variety of morphologies. In order to improve the interfaces between ZnO and hole-conducting polymers, routes to tune the length scales of the nanostructures are explored. We use SEM and AFM to investigate the surface morphology of ZnO, while the nanostructure inside the films can be probed with GISAXS. The understanding of the film morphology is helpful for improving the power conversion efficiency. The optical properties are examined with UV/Vis spectroscopy and the film thickness is investigated by x-ray reflectivity measurements.

CPP 11.4 Mon 18:15 Poster B2

Tuning the interface of hybrid thin films for PV applications — •Nuri Hohn[1], Lin Song[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. The major challenge to overcome the limited lifetime of such devices can be addressed via the substitution of an organic component with the respective inorganic counterpart for chemical/physical stability. Hence, a conjugated polymer serves as electron donor whereas n-type inorganic nanocrystals are deployed as electron conducting material. In such devices the surface-to-volume ratio is an indicator for both loss factors due to recombination as well as for efficiency gain through an increased amount of interface. Titanium dioxide nanostructures are obtained from sol-gel synthesis coupled with diblock copolymer templating to optimize the structure/interface between the donor and acceptor material. To improve the conditions for an efficient energy conversion in a PV cell primary investigations of the above mentioned systems correspond to spectral as well as morphological characterization via SEM and XRD.

CPP 11.5 Mon 18:15 Poster B2

Thermodynamic stability of mixed Pb:Sn methylammonium halide perovskites — •Ksenia Korshunova, Lars Winterfeld, Wichard J.D. Beenken, and Erich Runge — Institut für Physik und Institut für Micro- und Nanotechnologie, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Using density functional theory, we investigate systematically mixed $MA(Pb{:}Sn)X_3$ perovskites, where MA is $CH_3NH_3^+$, and X is I, Br or Cl. Ab initio calculations of the orthorhombic, tetragonal and cubic perovskite phases show that the substitution of lead by tin has a much weaker influence on both structure and cohesive energies than the substitution of the halogen. The thermodynamic stability of the $MA(Pb{:}Sn)X_3$ mixtures at finite, non-zero temperatures is studied within the Regular Solution Model.

We predict that it will be possible to create $MA(Pb{:}Sn)I_3$ mixtures at any temperature. This poster presents detailed numerical results supplementary to the results outlined in the talk given by our group.

CPP 11.6 Mon 18:15 Poster B2

Optoelectronic properties of mixed Pb:Sn methyl-ammonium halide perovskites — •Lars Winterfeld, Ksenia Korshunova, Wichard J.D. Beenken, and Erich Runge — Institut für Physik, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Using ab initio calculations, we investigate systematically the band structures of mixed $MA(Pb : Sn)X_3$ perovskites, where MA is $CH_3NH_3^+$, and X is Cl, Br or I. Here, we focus on the thermodynamically stable mixed structures in the high-temperature cubic phase and compare both DFT and post-DFT methods (including self-consistent GW) with and without spin orbit coupling. Interestingly, the optoelectronic properties are not just a linear combination of the non-mixed parent structures and are not limited by the non-mixed values, which allows band gap engineering. This poster presents detailed numerical results and a selection of over 150 different band structures supplementary to the results outlined in a talk given by our group.

CPP 11.7 Mon 18:15 Poster B2

Spectroscopic investigation of the nitrogen role in organic-inorganic perovskite films — •Małgorzata Sowińska[1], Chittaranjan Das[1], Konrad Wojciechowski[2], Henry Snaith[2], and Dieter Schmeisser[1] — [1]Brandenburgische Technische Universität Cottbus-Senftenberg, Angewandte Physik-Sensorik, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany — [2]Clarendon Laboratory, University of Oxford, Parks Road, Oxford, OX13PU, UK

Over the past few years, a wide range of device architectures employing organic-inorganic metal halide perovskite absorbers has been reported, with efficiencies exceeding 20%. Despite the tremendous progress, a number of key issues must be resolved before the wide-spread commercialization will be possible. Some of the primary challenges include lead toxicity, long-term stability, and fast degradation upon exposure to humid atmosphere. Recent computational and experimental studies suggest that hybrid metal-halide perovskites act as an ionic-electronic conductor. The study of vacancy-mediated migration of I^-, Pb^{2+} and $CH_3NH_3{}^-$ ions and their relative activation energies suggests that migration of halide vacancies, to and from the interfaces in the solar cell during its operation, is the main conduction mechanism. In this work, we are presenting high resolution synchrotron-based spectroscopic study, which indicates that the contribution of nitrogen into the conduction mechanism of methyl ammonium lead iodide-based ($CH_3NH_3PbI_3$) perovskite films should not be neglected. The N1s core level and resonant X-ray photoelectron spectroscopy at the N1s-egde of the $CH_3NH_3PbI_3$ films are discussed in detail.

CPP 11.8 Mon 18:15 Poster B2

Observation of ionic- and trapped charges at interfaces in an operating perovskite solar cell — •Victor Bergmann[1], Yunlong Guo[2], Hideyuki Tanaka[2], Ilka Hermes[1], Dan Li[1], Alexander Klasen[1], Simon Bretschneider[1], Eiichi Nakamura[2], Rüdiger Berger[2], and Stefan Weber[1,3] — [1]MPI for Polymer Research, Mainz — [2]University of Tokyo, Japan — [3]Johannes Gutenberg University Mainz, Germany

Optimization of solar cell devices requires efficient charge extraction. With cross section Kelvin probe force microscopy (KPFM), we were able to locally study the potential distribution inside a mesoporous device under working conditions (DOI:10.1038/ncomms6001). Here, we used frequency modulation KPFM to investigate cross sections of planar perovskite solar cells. In particular, we performed experiments in dark and under illumination on an operating planar $CH_3NH_3PbI_3$ device, in short circuit and open circuit conditions, respectively. Thereby, we found an experimental proof that both ion migration and trapped interfacial charges can be present in a perovskite device and demonstrate that cross sectional FM-KPFM is able to distinguish between the two effects.

CPP 11.9 Mon 18:15 Poster B2

Structure analysis on hybrid organic-inorganic perovskite solar cells — •Florian Soutschek[1], Harikesh P. Cholakkal[2], Sjoerd A. Veldhuis[2], Eva M. Herzig[1], Peter Müller-Buschbaum[3], Dharani Sabba[2], and Nripan Mathews[2] — [1]Technische Universität München, Munich School of Engineering, 85748 Garching, Germany — [2]Energy Research Institute @NTU (ERI@N), Research Techno Plaza, 637553, Singapore — [3]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

The desire to efficiently convert solar into electric energy has lead to increasing activity in the associated field of scientific research in the last decades. Due to major advantages, as low material costs and the applicability of mass production techniques, solution processsed solar cells have long been of particular interest; disadvantages such as comparatively low efficiency and fast degradation inhibited mass production so far. Combining advantages of organic and inorganic systems, perovskite solar cells - as hybrid organic-inorganic cells - have shown a skyrocketing rise in efficiency for the last years to currently around 20 %. However, little is known about the formation of the perovskite film under different conditions on a crystal size level, which is of key importance for the understanding of how to further improve this type of solar cells. Therefore the aim of this project is to use multiple measurement techniques, in particular Grazing Incidence Wide Angle X-ray Scattering (GIWAXS), on perovskite films with standard and systematically altered production procedures to learn about the film formation and possibilities of specific manipulation.

CPP 11.10 Mon 18:15 Poster B2

Fabrication and characterisation of solution processed perovskite solar cells with various transport layers — •Marvin Grüne[1], Stefan Väth[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

Perovskite solar cells are considered to be the upcoming star of thin film solar cells, exhibiting rapidly rising power conversion efficiencies (PCE). The active layer consist of the organic-inorganic perovskite structure $CH_3NH_3PbI_3$. The perovskite is sandwiched between a electron and hole transport layers which allows the selective extraction of the different types of charge carriers to the respective contacts of the solar cell. In this study different structures of solar cells, including different combinations of selective transport layers such as PEDOT:PSS and MoO_3 for hole transport or BCP, BPhen and Ca for electron transport were investigated concerning efficiency, hysteresis and long-term stability. Finally, the device stability of silver and gold as cathode material was inspected.

CPP 11.11 Mon 18:15 Poster B2

Revealing the structural properties of p-DTS(FBTTh$_2$)$_2$ with the help of MD-simulations — •Axel Bourdick and Stephan Gekle — Universität Bayreuth

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 unit are placed alternating on the same molecule.[1,2] With the help of MD-Simulations we simulate the system p-DTS(FBTTh$_2$)$_2$. In particular we investigate the structure and conformation of aggregated states in different solvents, and various physical properties, like the free energy of the system in dependence of the distance between molecules.

[1]: Gendron, D.; Leclerc, M. New Conjugated Polymers for Plastic Solar Cells. Energy Environ. Sci. 2011, 4, 1225-1237.

[2]: Duan, C.; Huang, F.; Cao, Y. Recent Development of Push-Pull Conjugated Polymers for Bulk- Heterojunction Photovoltaics: Rational Design and Fine Tailoring of Molecular Structures. J. Mater. Chem. 2012, 22, 10416-10434.

CPP 11.12 Mon 18:15 Poster B2

X-Ray Absorption Spectroscopy of Hybrid Organic-Inorganic Perovskites: Theory and Experiment — •C. Vorwerk[1], C. Hartmann[2], C. Cocchi[1], G. Sadoughi[3], S. Habisreutinger[3], R. Félix[2], R.G. Wilks[2,4], H. Snaith[3], P. Becker[2], J. Just[2], T. Unold[2], K. Hannewald[1,5], M. Bär[2,4,6], and C. Draxl[1,5] — [1]Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 14109 Berlin, Germany — [3]Clarendon Laboratory, Department of Physics, University of Oxford, Oxford OX1 3PU, United Kingdom — [4]Energy Materials In-Situ Laboratory Berlin (EMIL), Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany — [5]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany — [6]Institut für Physik und Chemie, Brandenburgische Technische Universität Cottbus-Senftenberg, 03046 Cottbus, Germany

We present a joint experimental and theoretical study of the x-ray absorption spectra (XAS) of the hybrid organic-inorganic perovskite methyl ammonium lead triiodide $CH_3NH_3PbI_3$ - a promising material for photovoltaic energy conversion. The Pb $M_{4,5}$ and I $L_{2,3}$ absorption edges of the perovskite were measured in partial fluorescence and total electron yield modes at the HiKE endstation located at the KMC-1 beamline of the BESSY II light source. The corresponding *ab-initio* calculations are performed using all-electron many-body theory (DFT+BSE), as implemented in the `exciting` code.

CPP 11.13 Mon 18:15 Poster B2

Impact of PbI_2 on excited state dynamics in hybrid lead halide perovskites — •Tobias Meier[1], Fabian Panzer[1,2,3], Tanaji Gujar[4], Thomas Unger[1,2], 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 have emerged as novel and highly efficient active material in different applications such as solar cells, or light emitting device. They also yield the possibility for cheap and simple processing which makes this class of material currently highly attractive and prominent. Depending on the processing method, it is known that PbI_2 incorporations can be present in the perovskite material after perovskite formation took place. Here a fundamental understanding on how and in which extend PbI_2 interacts with the perovskite domains and how this impacts on device performance is still missing. We therefore performed temperature dependent steady-state absorption and emission measurements, as well as transient absorption spectroscopy to investigate the impact of PbI_2 incorporations on the excited state dynamics in different $CH_3NH_3PbI_3$ samples.

CPP 11.14 Mon 18:15 Poster B2

Understanding excited state dynamics in hybrid lead halide perovskites by temperature dependent time resolved spectroscopy — •Marius Jakoby[1], Thomas Unger[1,2], 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

Within the last few years, hybrid lead halide perovskites have emerged as highly attractive active layers in solar cells and in light emitting devices. Here remarkably long charge carrier diffusion lengths in the range of several micrometers combined with the typically low binding energies of excited states are important material properties, which lead to high device efficiencies. Despite these high device efficiencies that were reported, there is still a lack in fundamental understanding the excited state dynamics of this class of material. For instance, there is still no clear consensus about the physical origin of additional emission features that are often observed at low temperature. To identify and characterise the dynamics of these different excited states we performed temperature dependent time resolved emission spectroscopy on different hybrid lead halide perovskite samples using a Streak-Camera setup. The results enable us to identify the nature of the different excited states and explore to which extend the morphology of the material controls their excited states dynamics.

CPP 11.15 Mon 18:15 Poster B2

X-Ray analysis towards highly stable, superior efficiency perovskite solar cells — •Shambhavi Pratap, Johannes Schlipf, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Perovskite solar cells represent the new wave in the field of photovoltaics and show a lot of promise. The technology has seen a meteoric rise with device performances crossing the 20% mark in just half a decade since its' inception.

The major challenge in the field remains the stability of these cells. The science of the response of the perovskite materials to atmospheric conditions of moisture and temperature demands considerable investigation before commercialization of these cells is feasible.

We aim to understand the structural changes occurring in the material with controlled humidity and temperature conditions, and to enhance the stability by the addition of functional additives and the use of novel solvent media during the synthesis of the perovskite crystals.

Grazing-incidence wide angle X-ray scattering (GIWAXS) aids us to understand the stability of the perovskite structure of the material and help us to gain insight for the fabrication of high-efficiency, long term stable perovskite solar cells.

CPP 11.16 Mon 18:15 Poster B2

Charge Extraction in Organometallic Perovskite Solar Cells — •Christian M. Wolff, Andreas Paulke, Natalie Schön, and Dieter Neher — Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str.24-25, D-14476 Potsdam-Golm, Germany

We present a study on transfer and extraction of charge carriers in working hybrid perovskite solar cells. With a toolbox comprising transient absorption (TAS), time-resolved PL (TRPL) and spectroscopic-electronic pump-probe experiments including time-delayed collection field (TDCF) and bias-assisted charge extraction (BACE) we follow the fate of charge carriers after excitation. We look at internal processes, such as recombination in the active layer, as well as external processes, such as extraction of charges to the transport layers. Whereas most previous studies have primarily investigated only sections of the solar cells, we apply the outlined techniques to working solar cells with all-organic (e.g. PEDOT and PCBM) or metal oxide (e.g. NiOx and ZnO) extraction layers. With these methods we gain insight into elementary processes in these high efficiency devices. For example, we find that electron transfer to PCBM occurs on a ns-time scale corresponding to mean extraction lengths of less than 20 nm. This finding is consistent with the interpretation, that PCBM molecules penetrate into the cracks between grains [1], in contrast to the picture of flat layers with sleek interfaces.

[1] Paulke, A. et al. Charge Carrier Recombination Dynamics in Perovskite and Polymer Solar Cells. Submitt. Publ. (2016).

CPP 11.17 Mon 18:15 Poster B2

Spectroscopic Imaging of Perovskites Thin Films — •Sebastian Baderschneider[1,2], Fabian Panzer[2,3], Thomas Unger[2,3], Tanaji Gujar[4], Mukundan Thelakkat[4], Jürgen Köhler[1,2], Anna Köhler[2,3], and Richard Hildner[1,2] — [1]Experimentalphysik IV, Universität Bayreuth — [2]Bayreuther Institut für Makromolekülforschung — [3]Experimentalphysik II, Universität Bayreuth — [4]Applied Functional Polymers, Makromolekulare Chemie I, Universität Bayreuth

The efficiency of perovskite solar cells has increased within a few years up to more than 20%. Responsible for the remarkable success of this class of solar cells are, among others, the high extinction coefficient over the whole visible range and low binding energies of the excited states allowing for efficient generation of charge carriers. Though mixed halide perovskites yield the possibility to be solution processed in a simple and cheap way, they show a high degree of crystallinity which ensures high diffusion lengths in the range of μm for both electrons and holes. Employing 2-dimensional spectroscopic imaging on thin polycrystalline perovskite films, we show that at low temperatures the crystal structure can be reversibly switched between the tetragonal and the orthorhombic phase. Moreover, we address the question whether the photoluminescence stems predominantly from the grain boundaries or the crystallites.

CPP 11.18 Mon 18:15 Poster B2

Charge Transport Properties in Perovskite Photovoltaic Devices Incorporating Carbon Nanotube Hole Transport Layers — Andrew Rowberg, Matthias Handloser, Kathrin Bader, Pablo Docampo, and •Achim Hartschuh — Ludwig-Maximilians-Universität München, München, Deutschland

Hybrid thin-film perovskite photovoltaic devices have attracted considerable interest due to their high efficiency and affordable fabrication. [1] However, the small molecule spiro-OMeTAD, the most often used hole transporting material in perovskite devices, suffers from a poor intrinsic charge mobility. Networks of semiconducting carbon nanotubes (s-CNTs), which possess excellent charge mobility properties, [2] offer a potential replacement and have been demonstrated as hole-transport layers in lead halide perovskite devices. [3] However, the mechanisms behind the functionality of perovskite devices incorporating s-CNT networks have not been thoroughly explored. This work examines the intrinsic charge transport properties in such devices through laser excitation at unique wavelengths corresponding to the absorption of each layers. A confocal optical microscope is used to raster-scan the samples or detection positions for fixed excitation and to generate photoluminescence (PL) maps, while charge carrier decay and transport dynamics are studied on the sub-nanosecond scale by time-correlated single photon counting (TCSPC) through rapid pulsed laser excitation.

[1] Hodes, G. et al. Nat. Phot. 8, 87-88 (2014). [2] Jariwala, D. et al. Chem. Soc. Rev. 42, 2824-2860 (2013). [3] Habisreutinger, S. et al. Nano Lett. 14, 5561-5568 (2014).

CPP 11.19 Mon 18:15 Poster B2

Ferroelectric organic layers for solar cell applications — •Malgorzata Wawrzyniak-Adamczewska[1] and Malgorzata Wierzbowska[2] — [1]Faculty of Physics, A. Mickiewicz University, Umultowska 85, 61-614 Poznan, Poland — [2]Institute of Physics, Polish Academy of Sciences (PAS), Al. Lotnikow 32/46, 02-668 Warszawa, Poland

Organic ferroelectric layers and molecular columns, arranged between the graphene sheets, are discussed for the solar cell application. The proposed layers possess many advantageous properties: 1) the cascade energy-levels alignment, 2) simultaneous donor and acceptor character depending on the charge-carrier direction, 3) the charge-transfer excitonic type, 4) the induced polarization of the electrodes, leads to a substantial work-function change (±1.5 eV) of the anode and cathode. The separate-path electron and hole transport is theoretically predicted for the layers and molecular columns. The carrier separation effect allows to deal with the charge recombination problem. The building molecules contain the mesogenic flat aromatic part and the terminal dipole groups which make the system ferroelectric. The diffusion path of the electrons cuts through the aromatic rings, while holes hop between the dipole groups. We verified that the separation of the diffusion paths is not destroyed by the application of the graphene leads. These features make the systems suitable for the efficient solar cells. (arXiv:1510.05220) This work has been supported by The National Science Centre of Poland: the Projects No.2013/11/B/ST3/04041 and DEC-2012/07/B/ST3/03412.

CPP 11.20 Mon 18:15 Poster B2

Crystalline Structure and Stability Studies of Differently Processed Hybrid Perovskite Films -Towards Stability under Ambient Conditions — •Tanaji Gujar and Mukundan Thelakkat — Applied Functional Polymers, Department of Macromolecular Chemistry I, University of Bayreuth, 95440 Bayreuth, Germany

Organic-inorganic halide perovskite-based thin film solar cells show excellent PCE. However, high PCE values have often been reached with poor air-stability. The degradation of its performance in moisture has attracted great attention, but the specific mechanism is not yet fully established. In this work, we used three different processing methods for the perovskite films preparation under N2 atmosphere and observed that the processing methods have a strong influence on the film structural properties and stability in ambient condition. Intensive characterizations including SEM, XRD and UV-Visible with aging of perovskite films in ambient conditions are carried out for understanding the structural and morphological relation with stability. Here we show that the films prepared by MAI-Vapor assisted method have compact, dense and pore-free with stability more than one month in ambient conditions. This also indicates that the formation of film morphology and structure could prevent water infiltration into the perovskite and increase the stability, thus enabling possibilities toward perovskite solar cells with long device lifetimes and a resistance to humidity. A comparison of the materials for their solar cell performance is also carried out. This work suggests important pathway to understand the degradation of the perovskite structure under normal humidity condition.

CPP 11.21 Mon 18:15 Poster B2

Effect of Thermal and Structural disorder on Electronic Structure of Hybrid Perovskite Semiconductor $\mathrm{CH_3NH_3PbI_3}$ — Cheng Li[1], Shivam Singh[2], K. L. Narasimhan[2], Fabian Panzer[3], Tanaji Gujar[4], Mukundan Thelakkat[4], Anna Köhler[3], Dinesh Kabra[2], and •Sven Hüttner[1] — [1]Organic and Hybrid Electronics, Makromol. Chemie I, Universität Bayreuth — [2]Indian Institute of Technology Bombay, Powai, Mumbai — [3]Experimentalphysik II, Universität Bayreuth — [4]Angew. Funktionspolymere, Makromol. Chemie I, Universität Bayreuth

We investigate the temperature dependence of optical properties of methylamonimum lead iodide ($\mathrm{MAPbI_3} = \mathrm{CH_3NH_3PbI_3}$) from room temperature to 6K. In both tetragonal (T> 163K) and orthorhombic (T<163K) phases of MAPbI3, the band gap decreases with decrease in temperature in contrast to what is normally seen for many inorganic semiconductors. We show that the temperature dependence of the band gap is determined by the lattice expansion term rather than 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 - reminiscent of Urbach tail absorption. The Urbach energy is a measure of the disorder, which is modelled using thermal and static disorder for both the phases separately. The static disorder component is small, which is consistent with the observed homogeneous broadening of the exciton with temperature. Both these features are a measure of the high crystal quality of the perovskite films.

CPP 11.22 Mon 18:15 Poster B2

Ion Migration in Perovskite based Solar Cells — •Cheng Li[1], Yu Zhong[1], Anna Gräser[1], Richard Hildner[2], and Sven Hüttner[1] — [1]Organic and Hybrid Electronics, Makromol. Chemie I, Universität Bayreuth — [2]Experimentalphysik IV, Universität Bayreuth

Solution processed Inorganic-organic halide organometal perovskite solar cells (e.g. $\mathrm{CH_3NH3PbI_3} - x\mathrm{Cl}_x$ and $\mathrm{CH_3NH3PbI_3}$) have demonstrated remarkable efficiencies recently. However, there is still a large space toward the theoretical limitation - the Shockley-Queisser Limit (33%). Hence, more and more interests are concentrated on factors which hinder the approach towards the limit. We employ different methods to especially address the issue of ion migration in perovskite based solar cells: electroabsorption (EA) spectroscopy explores the built-in potential in the working photovoltaic devices and temperature dependent dynamic processes are characterized by their current-voltage behavior in different temperatures. Furthermore, photoluminescence (PL) characterization, especially fluorescence microscopy (FM), is a powerful tool to investigate the trap states, excited states, charge carrier dynamics and etc., within the individual crystalline grains. We find that the PL blinking behavior in the whole film under the increasing intensity background. In addition, we also observe the process of PL decay during light illumination. We propose that this PL decay is associated with the migration of ions, especially the iodide ions, which are driven by the local electrical field induced by the light illumination.

CPP 11.23 Mon 18:15 Poster B2

Electric characterization of single crystalline and polycrystalline Copper-Zinc-Tin-Sulfide — •Martin Handwerg[1,2], Rüdiger Mitdank[1], Justus Just[2], Segej Levcenco[2], Thomas Unold[2], and and Saskia F. Fischer[1] — [1]AG Neue Materialien, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 14109 Berlin, Germany

Copper Zinc Tin Sulfide (CZTS) is investigated as absorption layer for solar cells to increase their efficiency. To understand the electrical transport mechanism in this material system, temperature dependent electrical conductivity measurements are carried out. Here, the temperature dependence of the electrical conductivity of single crystals and polycrystalline films is investigated. The composition of the polycrystalline films range from high copper (2.29 $n_{\mathrm{Cu}}/n_{\mathrm{Zn+Sn}}$) to low copper content (0.47 $n_{\mathrm{Cu}}/n_{\mathrm{Zn+Sn}}$), where as the single crystals have a stoichiometric composition. All measurements were performed between 4.2 K and 300 K and show an increase of conductivity with increasing temperature. Different hopping transport mechanism occur in different temperature regions: Nearest neighbor hopping at high temperatures, Mott variable range hopping at intermediate temperatures and Efros-Shklovskii hopping at low temperatures. Grain boundary scattering is detected in polycrystalline material as well. Also, the electrical conductivity increases with increasing copper content. Specific electrical applications can be designed by knowing these material properties.

CPP 11.24 Mon 18:15 Poster B2

Hydrothermal synthesis of methylammonium lead halide perovskites CH3NH3PbX3, (X = Br, Cl, I) — •Irina Anusca, Sabrina Iffländer, Samet Duman, Vladimir V. Shvartsman, and Doru C. Lupascu — Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Universitätsstraße 15, 45141 Essen, Germany

Compounds with organic-inorganic perovskite structure continues to be in the photovoltaic focus area because these materials have the abilities to combine the properties of inorganic part (high carrier mobility, wide range of bandgaps) and those of organic part (high efficiency luminescence, mechanical properties [1,2]. In the present work we report the preparation of the organic-inorganic perovskites CH3NH3PbX3, (X=Br, Cl, I) by low temperature (130°C) and autogenous pressure hydrothermal route and characterization by X-ray powder diffraction and optical UV-VIS spectroscopy. Keywords Hydrothermal synthesis; organic-inorganic perovskites; absorber solar cells Reference: [1]*KOJIMA, Akihiro ;TESHIMA, Kenjiro ; SHIRAI, Yasuo ; MIYASAKA, Tsutomu: Organometal halide perovskites as visible-light sensitizers for photovoltaic cells. In: Journal of the American Chemical Society 131 (2009), Nr. 17, S. 6050*6051 [2]*SNAITH, Henry J. ; ABATE, Antonio ; BALL, James M. ; EPERON, Giles E. ; LEIJTENS, Tomas ; NOEL, Nakita K. ; STRANKS, Samuel D. ; WANG, Jacob Tse-Wei ; WOJCIECHOWSKI, Konrad ; ZHANG, Wei: Anomalous Hysteresis in Perovskite Solar Cells. In: The Journal of Physical Chemistry Letters 5 (2014), Nr. 9, S. 1511*1515

CPP 12: Poster: Colloids and Complex Fluids

Time: Monday 18:15–21:00 Location: Poster B2

CPP 12.1 Mon 18:15 Poster B2

Aggregation behavior of doubly thermo-responsive polysulfobetaine-b-poly(N-isopropylmethacrylamide) diblock copolymers — •Natalya Vishnevetskaya[1], Viet Hildebrand[2], André Laschewsky[2], Peter Müller-Buschbaum[1], and Christine M. Papadakis[1] — [1]TU München, Physikdepartment, Physik weicher Materie — [2]University of Potsdam, Institute of Chemistry

Diblock copolymers consisting of a non-ionic poly(N-isopropylmethacrylamide) (PNIPMAM) block and a zwitterionic poly(sulfobetaine) (PSPP block) feature both a lower and an upper critical solution temperature (LCST and UCST) in aqueous solution. PSPP-b-PNIPMAM is expected to form (i) micelles with a PNIPMAM shell and a PSPP core or vice versa at low and high temperatures and (ii) unimers or large aggregates in the intermediate temperature range, depending on temperature, chemical structure and block length, as well as on the presence of electrolyte. The phase transition temperatures in dependence on the electrolyte concentration are investigated by turbidimetry. The aggregation behavior which is responsive to two stimuli (temperature and electrolyte concentration), and depends on the architecture of the non-ionic block, is studied by temperature-resolved small-angle neutron scattering (SANS) and dynamic light scattering (DLS). In D2O PSPP-b-PNIPMAM forms indeed micelles above the LCST and below the UCST. The micelle structures depend significantly on the block lengths, whereas the salt-induced changes are only minor.

CPP 12.2 Mon 18:15 Poster B2

Experimental study of Stokes Einstein relation for a colloidal particle in nonequilibrium viscoelastic media — •Johannes Berner[1], Juan Ruben Gomez-Solano[1], and Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universität Stuttgart, Germany — [2]MPI for Intelligent Systems, Stuttgart, Germany

Viscoelastic fluids are of great importance in biological systems and in medical and industrial applications. Their flow properties have been extensively studied by bulk rheology [1] and more recently by microrheology [2] using embedded colloidal probes. For instance in passive microrheology the Stokes Einstein relation is used to determine such properties by measuring the thermal fluctuations of the particle position [3]. This is only valid provided that the fluid and the particle are in thermal equilibrium. However this assumption is not trivially satisfied, if the microstructure of the fluid is driven far from equilibrium, e.g. by inducing a local deformation by means of the particle [4, 5]. In this work, we investigate the validity of the Stokes Einstein relation for a colloidal particle driven by optical tweezers through several viscoelastic media. In particular we focus on dependence on the local strain and strain rate.

[1] Larson R G 1999 The Structure and Rheology of Complex Fluids (New York: Oxford University Press), [2] Squires T. M. and Mason T. G., Annu. Rev. Fluid Mech., 42 (2010) 413, [3] Mason T. G. and Weitz D. A., Phys. Rev. Lett., 74 (1995) 1250, [4] Gomez-Solano J. R. and Bechinger C., EPL, 108 (2014) 54008, [5] Gomez-Solano J. R. and Bechinger C., New J. Physics, 17 (2015) 103032

CPP 12.3 Mon 18:15 Poster B2

Interactions of self-propelled micro-swimmers in viscoelastic fluids. — •Mahsa Sahebdivani[1], Juan Ruben Gomez-Solano[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 micro-swimmers, such as bacteria and spermatozoa, commonly takes place in viscoelastic fluids and in complex crowded environments. Contrary to the extensive studies on the motion of artificial micro-swimmers in Newtonian fluids [1], only in a few experimental works, the swimming mechanism of some microorganisms e.g. algal cells [2], and E. coli [3] has been done. In our work, we experimentally investigate the motion of spherical Janus particles in viscoelastic fluids with very large relaxation times. In particular, we focus on the behavior of these active particles in presence of walls and obstacles, where very long-range interactions are mediated by the transient flow fields induced by the active motion of the micro-swimmers [4]. We also study inter-particle interactions between micro-swimmers, where the viscoelasticity of the surrounding fluid gives rise to dramatic differences in their collective behavior compared to the motion in Newtonian fluids.

[1] I. Buttinoni, et al., J. Phys.: Cond. Mat. 24, 284129 (2012) [2] B. Qin, et al., Sci. Rep. 5:9190 (2015) [3] A. E. Patteson, et al., Sci. Rep. 5:15761 (2015) [4] Gomez-Solano. , Bechinger, New J. Phys. 17(2015)103032

CPP 12.4 Mon 18:15 Poster B2

Discontinuous thinning behavior in active microrheology of attractive colloids — •Robert Wulfert[1], Udo Seifert[1], and Thomas Speck[2] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany

Arguably the most exciting phenomena in traditional macrorheology hinge on the non-linear response of complex fluids to external flows. In extreme cases, non-linear flow curves can even comprise discontinuities, as in the paradigmatic example of cornstarch suspensions, which solidify abruptly when exceeding a certain critical strain-rate. Active microrheology (AMR) has established itself rather recently as a complementary approach to infer viscoelastic properties of complex media by driving an embedded colloidal probe and tracing its microscopic trajectory. Although the existence of an exact relation between micro- and macrorheology remains an open issue, AMR has qualitatively reproduced quintessential properties like the thinning and thickening of colloidal soft-matter under flow. Based on the well-established *simple-paradigm* model for AMR, we report on discontinuous force-thinning of colloidal suspensions with attractive long-range interactions: At a critical force, the suspensions microviscosity drops abruptly by about an order of magnitude. By complementing numerical solutions of the pair-Smoluchowski equation with Brownian-dynamics simulations, hysteretical behavior around this critical force is revealed for finite-time force protocols.

CPP 12.5 Mon 18:15 Poster B2

Simultane Bestimmung von Statik, Elastizität und Dynamik an einem Hart-Kugel-Yukawa System — •Sabrina Heidt — Institut für Physik, JGU, D-55099, Mainz, Deutschland

Anhand eines Hart-Kugel-Yukawa Systems wird die simultane Messung von statischen, elastischen und dynamischen Eigenschaften am selben Ensemble mit einer Kombinationslichtstreuanlage (SED) demonstriert. Da die Eigenschaften eines kolloidalen Festkörpers sowohl von den Präparationsbedingungen als auch von der Mikrostruktur der Probe abhängen, eignet sich der vorgestellte Messaufbau besonders zur Vermeidung von transportbedingten Einflüssen auf das Messergebnis. Die im Eigenbau konstruierte SED besteht aus einer statischen, einer dynamischen Lichtstreuanlage und einer Torsionsresonanzspektroskopie zur Schermodulbestimmung kristalliner Proben. Bei dem verwendeten Probensystem aus 80 nm großen Poly-n-Butylacrylamid-co-Polystyrol Kolloiden (PnBAPS80) kann in Abhängigkeit von der Partikelanzahldichte und der Salzkonzentration eine kubisch raumzentrierte Kristallstruktur beobachtet werden. Wobei gleichzeitig das Phasenverhalten und die Kristallisationskinetik wie auch das Schermodul bestimmt werden können. Charakteristische Eigenschaften zur Beschreibung des Systems sind dabei Kolloidgrößen, Kristallitgrößen, Nukleationsraten und Oberflächenspannungen. Durch den Vergleich der präsentierten Ergebnisse der PnBAPS80 mit Literaturdaten anderer kolloidaler Systeme, soll die Leistungsfähigkeit der Anlage verifiziert werden.

CPP 12.6 Mon 18:15 Poster B2

Colloids trapped at fluid interfaces: Capillary-driven dynamics for binary mixtures — •Malte Lütje, Martin Oettel, and Johannes Bleibel — Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen

We investigate a binary system of micron-sized colloids that are trapped at liquid-liquid or liquid-gas interfaces. The deformation of the interface due to external forces (i.e. gravity) acting on the colloids gives rise to long-ranged, logarithmic capillary attractions. For a wide range of parameters, these attractions render the system unstable: An initially homogeneous distribution of the colloids on the surface will collapse.

We perform Brownian Dynamics simulations of this system. Interactions between colloidal particles are implemented through a short-ranged repulsion and capillary interactions which dominate the dynamics on different length scales, respectively. We study the dynamical properties and conditions for stability.

As the capillary interactions strongly depend on the radius of the particles, the system and its dynamical phase diagram change if we introduce a second species of smaller colloids. We study the impact of the second species on stability and provide simulation results for the capillary collapse using various sets of parameters.

CPP 12.7 Mon 18:15 Poster B2

The non-equilibrium process of the porous polymer film formation: modeling — •Masoud Amirkhani, Farid Farajollahi, and Othmar Marti — Institut für Experimentelle Physik, Universität Ulm

The breath figure (BF) is a very wide spread method for fabricating porous polymer film. The BF is a simple method, which one uses the condensation of water on an evaporating surface of polymer solution to produce porous film or porous surface. In spite of the simplicity of the BF technique, there is not a physical model that can describe the process. This is due to the complexity of the process, which includes evaporation of the solvent, condensation of water droplets, emerging droplets, mass and heat convection. The combination of the mentioned phenomenon leads to a complicated non-equilibrium process that is very sensitive to the initial system parameters (such as polymer concentration, solvent, the structure of polymer and etc.) and environmental condition (such as temperature, humidity, substrate, airflow speed and etc.). In this work, we describe a possible road map to model the BF and understand the mechanism behind the formation of regular honeycomb structure on the surface of the polymer.

CPP 12.8 Mon 18:15 Poster B2

Influence of Polymer Brush Coated Substrate on the Active Motion of Janus Particles — •Mojdeh Heidari, Stefan Wellert, and Regine von Klitzing — Stranski Laboratorium für Physikalische und Theoritische Chemie, Inst. für Chemie TU Berlin, Straße des 17. Juni, 10623 Berlin, Germany

Au-polystyrene Janus particles demonstrate a thermophoretic induced motion under laser illumination (λ=532 nm). In this study we explore the 2D self-propulsion of Janus particles between two glass substrates. The substrate is functionalized with polymer brushes, as it is hypothesized that the lubricative nature of brushes will reduce the friction coefficient of the substrate which subsequently has a significant influence on the motion of particles close to the substrate. Hence, polymer brushes with varied grafting densities and thicknesses have been synthesized and the corresponding elastic properties have been characterized using colloidal probe AFM. Trajectories of particles are represented under different laser intensities.

CPP 12.9 Mon 18:15 Poster B2

Preparations for DCMIX-3: data analysis from SODI experiments aboard the ISS — •Thomas Triller and Werner Köhler — Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany

The ISS offers a unique environment for experiments which require microgravity on long timescales. Especially thermodiffusive processes in multicomponent mixtures can be difficult to measure on earth, due to gravitational instabilities. Therefore, a collaboration of several international teams aims to establish within the framework of the ESA DCMIX project a set of reliable benchmark data for selected ternary fluid mixtures measured aboard the ISS. These experiments are done with SODI (Selectable Optical Diagnostics Instrument), a Mach-Zehnder interferometer. The resulting interferograms contain data about the local refractive index, and therefore the local composition of the fluid, across the whole sample cell (also called thermodiffusion cell). The refractive index can be extracted from the interferograms via a Phase Unwrapping method. The DCMIX-3 experiment (the system Water/Ethanol/Triethylene-glycol) was scheduled to fly to the ISS in October 2014. Unfortunately, a catastrophic failure during takeoff destroyed all samples aboard the Orb3 transport. A new flight is planned for April 2016. In the meantime, data from the previous DCMIX-1 experiment (Dodecane/Isobutylbenzene/Tetralin) allow to verify the analysis methods which were implemented for DCMIX-3. These methods make use of the fundamental similarity of all optical experiments involving a thermodiffusion cell.

CPP 12.10 Mon 18:15 Poster B2

Adsorption of silver complexes on gold nanorods - a combined SAXS/SANS study — •Tilo Schmutzler, Torben Schindler, and Tobias Unruh — Friedrich-Alexander-University Erlangen-Nuernberg, Chair for Crystallography and Structural Physics, Staudtstrasse 3, 91058 Erlangen, Germany.

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

The synthesis of Au nanorods (AuNRs) includes the addition of AgNO3 as catalytic component. The exact role of the silver species during the rod formation is rather unclear.

Using small angle neutron scattering (SANS) we were able to proof the adsorption of silver complexes on the gold nanorod surface. Thereby the AuNRs were stabilized by the micelle forming surfactant CTAB (Cetyltrimethylammonium bromide). SANS is very sensitive to the existence of these micelles due to the large scattering contrast in D2O whereas small angle X-ray scattering (SAXS) can be used to characterize the AuNRs itself. By the addition of AgNO3 and thiourea into a AuNR solution (1mM CTAB) the release of CTAB micelles was proofed by the increased neutron scattering related to the micelles. So far, we assume that the silver thiourea complexes replace the CTAB molecules at the AuNR facets resulting in the formation of micelles.

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

CPP 12.11 Mon 18:15 Poster B2

Self-Assembly in Dipolar Fluids — •Michela Ronti and Sofia Kantorovich — University of Vienna, Austria

We study low temperature and low density phase behaviour of Dipolar Hard Spheres (DHS) systems. From a theoretical point of view the process of self-assembly is not responsible for a phase transition; this belief was completely reverted by theoretical studies showing that the process of self-assembly is alone capable to induce phase transition(1). On the other hand in the last years it was proved that no sign of critical behaviour is observed, implementing efficient and tailored Monte Carlo algorithms(2). Moreover a theoretical approach based on Density Functional Theory was developed: a series of structural transitions were discovered providing evidence of a hierarchy in the structures on cooling (chains, rings, branched structures)(3). We perform free-energy calculations in order to draw the phase diagram of DHS model. Comparing the numerical results with the theoretical ones shed light on the scenario of temperature induced structural transitions in magnetic nano colloids.

(1) T.Tlusty and S.A.Safran, Science 290 (2000) (2) L.Rovigatti, J.Russo and F.Sciortino, Soft Matter 8 (2012) (3) S.S.Kantorovich, A.O.Ivanov, L.Rovigatti, J.M.Tavares and F.Sciortino, Phys. Chem. Chem. Phys. 17, 16601 (2015)

CPP 12.12 Mon 18:15 Poster B2

Investigations on the kinetics of Liquid-Liquid Phase Separation and dynamic arrest in protein systems — •Stefano Da Vela[1], Fajun Zhang[1], Alessandro Greco[1], Michael Sztucki[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

Aqueous solutions of bovine γ-globulin in the presence of polyethylene glycol, and of bovine serum albumin in the presence of Yttrium(III),are studied in comparison as two widely differing protein systems, both featuring Liquid-Liquid Phase Separation (LLPS). While in bovine γ-globulin LLPS is determined by an isotropic attractive depletion interaction, in bovine serum albumin LLPS is triggered by Yttrium cations activating a directional "patchy" attractive interaction. Notably, while for γ-globulin the LLPS boundary has an upper critical solution temperature, albumin features a lower critical solution temperature behaviour. The experiments focus on the kinetics of phase separation in samples at high protein volume fraction, driven in the two phase regime by a rapid temperature variation. The development of μm size structures is followed through the stages of the phase separation by state-of-the art time resolved Ultra Small Angle X-Ray Scattering (USAXS) and time resolved Very Small Angle Neutron Scattering (VSANS), complemented by optical microscopy. The time evolution of the characteristic length and the analysis of the scattering profiles allow for a comparison between the two systems and for interpretation of the data relative to the later stages of the phase separation.

CPP 12.13 Mon 18:15 Poster B2

manipulating the assembly of wet-deposited nanocolloids based on in situ GISAXS study — •Peng Zhang[1,2] and Stephan Roth[1] — [1]Deutsches Elektronen-Synchrotron (DESY), Notkestrasse 85, D-22607 Hamburg, Germany — [2]Leibniz Institut für Neue Materialien, Campus D2 2, 66123 Saarbrücken, Germany

The assembly of the nanoparticles and formation of ordered structure during solvent evaporation is strongly influenced by the environmental factors like temperature, surfactant and interface interaction. How to track in situ the kinetic process of nanoparticle assembly is vital for the achievements of structure ordering and optimized functionality. This work reports an in situ study of the assembly process of polystyrene nanocolloids by a smartly designed toolkit, combining the nanocolloidal thin film preparation with air-brush spray deposition and structure analysis with grazing-incidence small angle X-ray scattering (GISAXS). The homogeneously dispersed nanocolloidal thin film is successfully prepared with manipulating the solvent evaporation rate. This is contrast to the generally reported inhomogeneous deposition of particles, e.g., "coffee-ring" like structure. By a qualitative analysis, the inhibition of nanocolloidal aggregation is rationalized by the fact that the necessary diffusion time of most adjacent two nanocolloids is longer than the drying time. This finding is expected to be helpful for the fast fabrication of wet-deposited nanocomposite in thin film.

CPP 12.14 Mon 18:15 Poster B2

The behavior of individual supramolecular ferromagnetic filaments and their suspensions — •Ekaterina Novak[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

Self-assembly in polymer and colloid systems has acquired a special significance nowadays in the context of the development of new smart materials. Here we present the investigation of individual supramolecular ferromagnetic filaments and their suspensions. Filaments are an analogue of a macromolecular polymer, where magnetic nanoparticles are playing a role of predetermined shape monomers. Our research is focused on the setting and analysis of molecular dynamics computer simulation for linear and circle shapes ferromagnetic filaments with dipole hard spheres. We would aim at investigating end-to-end distance, radius of gyration, the self-organization of these filaments, the interaction potentials. Additionally we give a detailed comparison of the behavior of suspension of ferromagnetic filaments and ferrocolloids. These results will form the basis of theoretical models and recommendations on the synthesis of new materials.

CPP 12.15 Mon 18:15 Poster B2

The self-diffusion coefficient in the magnetic fluids — •Alla Dobroserdova[1] and Sofia Kantorovich[1,2] — [1]Ural Federal University, Lenin av. 51, Ekaterinburg, 620000 Russia — [2]University of Vienna, Sensengasse 8, 1090 Vienna, Austria

We present the results on the self-diffusion coefficient in the systems of magnetic dipolar particles. Of course, there were some attempts to study diffusion [Yu. A. Buyevich et al., Physica. A 190, 276 (1992); P. Ilg, Phys. Rev. E 71, 051407 (2005); J. Jordanovic et al., Phys. Rev. Lett. 106, 038301 (2011)], but the detailed theoretical description is still missing. We consider the ferrofluids with chain aggregates of dipolar spheres in the three-dimensional case and with chains and rings in the quasi-two-dimensional one. We can study how the self-diffusion coefficient depends on the system polydispersity, granulometric composition, geometrical constraints and dipolar stregths. In our study, we combine theoretical approach and computer simulation. In theoretical study, we use Density Functional Approach to obtain the chain and ring concentrations. Then we can use them to obtain the self-diffusion coefficients. Also we perform molecular dynamics simulations. We compare theoretical results and data of the computer simulations and we have good agreement.

CPP 12.16 Mon 18:15 Poster B2

Depletion interaction potentials for linear and ring polymer chains in a solution of mesoscopic colloidal particles of big size — •Piotr Kuterba[1] and Zoryana Usatenko[2] — [1]Jagiellonian University, Cracow — [2]Institute of Physics, Cracow University of Technology, Cracow

Investigations of a dilute solution of linear and ring polymer chains immersed in a confined geometry of two mesoscopic colloidal particles of big size and between wall and colloidal particle for different boundary conditions, such as: Dirichlet-Dirichlet, Neumann-Neumann and Dirichlet-Neumann which correspond to the situation of two repulsive walls, two inert walls and for the mixed case of one repulsive and one inert wall were performed. Taking into account the well known polymer - magnet analogy developed by de Gennes and Derjaguin approximation for the case of big colloidal particles the calculations of the correspondent depletion interaction potentials were performed for all above mentioned cases. The obtained results indicate, that introducing the curvature for two surfaces leads to the reducing of the correspondent depletion interaction potentials. The obtained results are in good qualitative agreement with previous theoretical investigations.

CPP 12.17 Mon 18:15 Poster B2

Investigation of the anisotropic magnetic particle systems with moderate and high concentrations — •Elena Pyanzina[1] and Sofia Kantorovich[1,2] — [1]Ural Federal University, Lenin av. 51, Ekaterinburg, 620000, Russia — [2]University of Vienna, Sensengasse 8, Wien, 1090, Austria

Nowadays, anisotropic magnetic particles form the cutting edge of dipolar soft matter research as they correspond completely to the idea of fine tuning and designing new materials with controllable microstructure. As a result, various microproperties can be tuned via changing the particles concentration and the particles properties. In this contribution we focus our attention on the influence of the particles' concentration on the different system properties. The theoretical study and results of computer simulations for microstructure and magnetic, rheological and structural properties of the concentrated systems with different particle shape anisotropy and dipole orientation inside the particle are presented. It was shown that all aforementioned characteristics depend on the particles concentration and particles' parameters. This may prove to be very important in various medical and industrial applications, where a bottom up design of materials plays a crucial part.

CPP 12.18 Mon 18:15 Poster B2

The dynamical phase diagram of the capillary attraction induced collapse of colloidal monolayers at fluid interfaces — Johannes Bleibel[1], Alvaro Domínguez Alvarez[2], •Hans Joachim Schöpe[1], and Martin Oettel[1] — [1]Eberhards Karls Universität Tübingen, Auf der Morgenstelle 10, 72026 Tübingen, Germany — [2]Física Teórica, Universidad de Sevilla, Apdo. 1065, 41080 Sevilla, Spain

We investigate the evolution of a system of colloidal particles, trapped at a fluid interface and interacting via capillary attraction in theory, simulation and experiment. We address the clustering behavior of an initially homogeneous particle distribution and the collapse of a radially symmetric distribution of finite size. It investigated both theoretically by using a perturbative approach inspired by cosmological models and numerically by means of Brownian dynamics (BD) and dynamical density functional theory (DDFT). Furthermore our investigation includes hydrodynamic interactions. We find an accelerated dynamics in the collapse regime. The qualitative phenomenology summarized in the dynamical phase diagram however, remains unchanged. Colloidal particle about 20 micrometer in size trapped at a water decane interface serve as the experimental counterpart. Particles trajectories can easily monitored by bright field microscopy. This allows a direct comparison between theory and experiment.

CPP 13: Poster: Nanoparticles, Nanocrystals and Composites

Time: Monday 18:15–21:00 Location: Poster B2

CPP 13.1 Mon 18:15 Poster B2

Study of silica nanoparticles/polymer hydrogel nanocomposite — •Elsa Perrin[1,2], Martin Schoen[1,3], and Anne Boutin[2] — [1]Stranski-Laboratorium für Physikalische und Theoretische Chemie, Fakultät für Mathematik und Naturwissenschaften, Technische Universität Berlin, Berlin, Germany — [2]Ecole Normale Supérieure, PSL Research University, UMR PASTEUR, Paris, France — [3]Department of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, North Carolina, USA.

The design of nanocomposite materials is a fast-growing field with many novel and exciting materials such as nanocomposite polymer hydrogels. In particular, the coupling between the chemistry of adsorption and the resulting mechanical properties has been poorly explored. Recently a way has been found to glue together two polymer gels using nanocomposite materials made by polymers and silica nanoparticles (NPs). It is proposed for the first time that spreading a droplet of a silica NP solution on the surface of one gel and then bringing a second gel into contact with it leads to strong adhesion between the two gels.

However, the interaction between the polymer network and the NPs is still not well understood. Modeling the interactions between polymers and silica particles at the quantum level, using density functional theory, will allow us to get insight into the adsorption energy of the polymers on the NPs surface. Moreover, studying this system with coarse-grained molecular dynamics simulations will give us information about the organization of the polymer chains around the silica NPs.

CPP 13.2 Mon 18:15 Poster B2

Porous titania-based hybrid films as electrodes for lithium-ion batteries — •Thomas Kaps, Ezzeldin Metwalli, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Porous titania films are promising candidates as electrodes for lithium-ion batteries. Large surface area of nanoporous titania films enables both, high current density and improved cycling behavior. Sol-gel templating is nowadays a widely used technique to create nanoscale porous structures. PS-b-PEO diblock copolymer is used as a structure directing agent to create foam-like mesoporous titania/silicon composite films via sol-gel method. The morphology of the porous hybrid films was probed with SEM, X-ray diffraction and GISAXS. The crystallinity of the titania films was systematically measured as a function of the silicon nanoparticle content following the calcination step at different temperatures. The titania/silicon hybrid films are tested as electrodes for lithium-ion batteries showing a unique combination of both, the high capacity and the resistance to the lithium dendrites formation.

CPP 13.3 Mon 18:15 Poster B2

Printed nanostructured block-copolymer/metal-oxide hybrid films — •Senlin Xia, Ezzeldin Metwalli, Yuan Yao, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Metal-polymer nanocomposites are important hybrid materials due to their interesting applications, e.g. catalysts, sensors, and memory devices. Owing to the potential of high mass production and energy saving, printing techniques were utilized to prepare hybrid films composed of magnetite nanoparticles (NPs) and PS-b-PMMA diblock copolymer (DBC). Different 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 parallel lamella NP-DBC 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 13.4 Mon 18:15 Poster B2

Magnetic properties and structure of block copolymer-cobalt oxide nanocomposite thin films — •Hong Xu, Ezzeldin Metwalli, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Nanostructured polymer-metal oxide composites are a current research area of great importance due to its highlight applications in sensors, optics and catalysts. In the present investigation, the structure and properties of hybrid films composed of a PS-b-PMMA diblock copolymer (DBC) and cobalt metal salt were investigated. Cobalt metal salt oxidation in the polymer matrix was probed with UV/Vis and FTIR spectroscopies during the thermal treatment step. The interdomain lamella spacing D was evaluated using GISAXS as a function of cobalt salt concentration. The D values increased with an increasing of Co/PMMA molar ratios. Both, paramagnetic and superparamagnetic behavior of the heat-treated hybrid films were proved at different cobalt salt contents using superconducting quantum interference device magnetometer.

CPP 13.5 Mon 18:15 Poster B2

Numerical studies of acoustic metamaterial multilayers — •Takamichi Terao — Gifu university, Gifu, JAPAN

The vibrational properties of acoustic metamaterial multilayers, which are made of a periodic arrangement of clusters of mass and mass-in-mass microstructure, were numerically studied. The dispersion relations of one-dimensional multilayers and two-dimensional periodic structures with square lattices were clarified. It was confirmed that flat modes appear in a sonic band gap, and that the number of such in-gap modes can be controlled by changing the structure of a multilayer. The physical origin of the flat modes is also discussed.

CPP 13.6 Mon 18:15 Poster B2

Strong correlated electronic system in Mn3+ oxide revealed by RIXS — •Daniela Schön, Ronny Golnak, Marc F. Tesch, Jie Xiao, and Emad F. Aziz — Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Deutschland

MnOx has been demonstrated as effective water oxidation catalysts, among which Mn3+ species has been proven as the most efficient ingredient when compared to other Mn oxidation states. The information on electronic structure of MnOx is certainly critical to understand the catalytic mechanism and to further improve the catalytic activity. While most of the electronic structure investigations are conducted on solid samples, few are performed in liquid environment to mimic realistic conditions. We selected solvated Mn3+acac3 in dichloromethane as a prototypical system to carry out in-situ RIXS measurements, an ideal model system probed by a proper technique. Mn3+ ion is coordinated by six O atoms in liquid phase, which perfectly simulates the situation of Mn3+ species during water catalysis. RIXS is able to detect element-specific valence excitations in bulk, an ideal tool to probe local (catalytic site) electronic structure of Mn in liquid. Moreover, the intensity ratio of RIXS loss features to normal emission features can be utilized to determine the extent of the electronic correlation in the target system. Intense RIXS loss features of Mn3+ are observed, implying a highly localized and strong correlated electronic system in Mn3+ d4 configuration.

CPP 13.7 Mon 18:15 Poster B2

Molecular Dynamics Simulations of a Peptide Modified Silica Nanopore — •Kai Stroh, Julian Geske, and Michael Vogel — Institut für Festkörperphysik, TU Darmstadt

The combination of biological and synthetic nanopores is of great biotechnological interest. While being highly selective and sensitive, biological nanopores lack the robustness for technological applications. In contrast silica pores are well-proven in industrial and clinical environments, but possess inferior capabilities, e.g. no selectivity. A hybrid system would combine the favourable properties of both fields.

To investigate the interactions between biological chain molecules attached to mesoporous materials and various liquids, we employ molecular dynamics simulations. For our peptide modified silica system we chose a slit pore geometry. Elastin-mimetic peptides $(\mathrm{VPGVG})_n$ are grafted onto the two surfaces of a silica slab via suitable linker molecules. The intergallery space is filled with aqueous mixtures. We study how the configuration of the peptide changes in the vicinity of a silica surface and how the behavior of the water mixtures is affected by the confinement. Moreover, we investigate the dynamical couplings of peptide and solvent molecules.

CPP 13.8 Mon 18:15 Poster B2

Mechanical properties of molecularly covered silver nanowires investigated by SFM — •Katherine A. Herman[1], Egon Steeg[1], Jürgen P. Rabe[1,2], and Stefan Kirstein[1] — [1]Department of Physics, Humboldt Universität zu Berlin — [2]IRIS Adlershof, Humboldt Universität zu Berlin

Silver nanowires with uniform diameters of 6.5 nm were deposited onto solid substrates and investigated using scanning force microscopy (SFM). The wires were synthesized using an established protocol[1] with a soft tubular molecular aggregate template in aqueous solution. Filled and unfilled tubule segments could best be discriminated by the phase contrast of the intermittent contact SFM imaging mode. Contact mode SFM was used to move, bend and break deposited tubules with and without silver wires. Analysis of the broken and dragged segment lengths suggests that the wires break preferentially at certain grain boundaries, as expected for a polycrystalline material. Analysis of the wire conformations indicates that the wires were plastically deformed during deposition.

[1] D. M. Eisele, H. v. Berlepsch, C. Böttcher, K. J. Stevenson, D. A. Vanden Bout, S. Kirstein, J. P. Rabe. *J. Am. Chem. Soc.*, 2010, 132**(7)**, pp 2104-2105.

CPP 13.9 Mon 18:15 Poster B2

Novel Growth Mechanism of ZnO Hexagonal Microtube Optical Resonators — •Jinxin Zhan[1], Hongxing Dong[1], Shulin Sun[2], Xiaodong Ren[3], Jianjun Liu[3], Zhanghai Chen[2], Chritoph Lienau[4], and Long Zhang[1] — [1]Shanghai Institute of Optics and Fine Mechanics, 201800 Shanghai, China — [2]Fudan University, 200433 Shanghai, China — [3]Shanghai Institute of Ceramics, 200050 Shanghai, China — [4]Carl von Ossietzky Universität, 26111 Oldenburg, Germany

Tubular micro/nanostructures have gained considerable interest for both fundamental scientific studies and practical applications due to their unique and delicate constructions [1-2]. However, for quite a long time, it was quite difficult to synthesize tubular structures for non-layered materials such as oxides, metals and nitrides because of the difficulties of controlling their dimensions.

Here we observed a novel growth mechanism of tubular ZnO microstructures. As demonstrated by a detailed growth study of ZnO crystals and by first-principles calculations, the formation of H_2/H_2O vapour changes the ZnO crystal surface energy and controls the geometry of ZnO micro/nanotubes.Furthermore, we demonstrated that the fabricated microtubes could be employed as tunable optical resonators. The effect of the unique tubular structure on the intensity modulations is discussed theoretically based on a plane wave model and finite-element-method (FEM) simulations, which agrees well with the experimental results.

[1] J. Xu et al., Adv. Mater. 26, 5337 (2014); [2] H. X. Dong et al., J. Mater. Chem. 20, 5510 (2010)

CPP 13.10 Mon 18:15 Poster B2

Studying visible-light photodegradation of Benzidine azo dye on Titanium dioxide nanotubes using Surface Enhanced Resonance Raman Spectroscopy — •Christine Joy Querebillo[1,2], Hoang Khoa Ly[1], Ibrahim-Halil Öner[1], Ulrich Gernert[3], Peter Hildebrandt[1], and Inez Marita Weidinger[1] — [1]Institut für Chemie, PC 14, Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany — [2]School of Analytical Sciences Adlershof, Humboldt-Universität zu Berlin, IRIS Building, Unter den Linden 6, 10099, Berlin, Germany — [3]Zentraleinrichtung Elektronenmikroskopie (ZELMI), Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany

Surface Enhanced Resonance Raman Spectroscopy (SERRS) is used to study the photodegradation of an azo dye pollutant, Benzidine-p-aminothiophenolate (BD-PATP), on Titanium dioxide (TiO2) nanotubes. Unlike many degradation studies on TiO2 which use UV light, here, we use visible light to photodegrade BD-PATP on TiO2 of different surface enhancements achieved with different post-anodization heat treatment temperatures (300-500°C). Heating the TiO2 nanotubes at these temperatures improves the crystallinity, as seen in Raman, and affects the morphology of the nanotubes, as seen using scanning electron microscopy.

SERRS was used to confirm the synthesis of BD-PATP on TiO2 from PATP on TiO2 and to monitor the photodegradation of BD-PATP on TiO2. For the latter, we infer on the effect of the surface enhancement of the nanotubes on the photodegradation kinetics.

CPP 13.11 Mon 18:15 Poster B2

Highly efficient energy transfer from quantum dot to allophycocyanin in hybrid structures — •Anastasia Karpulevich[1,3], Evgeny Maksimov[1], Nikolay Sluchanko[2], Alexandr Vasiliev[1], and Vladimir Paschenko[1] — [1]Lomonosov Moscow State University, 119991, Moscow, Russia — [2]A.N.Bach Institute of Biochemistry, 119071, Moscow, Russia — [3]Institute of Physical Chemistry, Hamburg University, 20146, Hamburg, Germany

Development of light-energy converters based on photosynthetic mechanisms is one of the promising directions in modern biophysics. Quantum dots can be used as a substitution to the native light-harvesting antennae, increasing absorbtion cross-section of purified photosystem as a result of non-radiative energy transfer [1]. We investigated model system consisting of CdSe/ZnS core-shell quantum dot (QD) and protein allophycocyanin (APC). Using spectroscopic methods we shown that QD-APC hybrid systems are able to self-assemble in solution. We found that steric accessibility plays a key role for the energy transfer: the energy migration efficiency in hybrid structures reaches 90 % for APC monomers and only 30 % for trimers. Additionally, we obtained stable covalently bound QD-APC hybrids. We observed considerable amplification of APC fluorescence in the optical range of excitation between 400 and 500 nm, where QD absorption prevails. The results might be used for the creation of bright and stable fluorescent dyes based on allophycocyanin.

[1] E.G. Maksimov et al., Biochem., vol. **77**, no. 6, pp. 624*630 (2012).

CPP 13.12 Mon 18:15 Poster B2

Scanning aperture trapping of nanoparticles for plasmonic enhancement of fluorescence — •Yazgan Tuna, Ji Tae Kim, and Vahid Sandoghdar — Max-Planck-Institute for the Science of Light, 91058 Erlangen

Trapping and manipulation of small objects have been of interest for a range of applications. Here we report on an electrostatic trap that is created in an aqueous medium between the aperture of a nanopipette and a glass substrate without the need for external potentials. Furthermore, we demonstrate scanning aperture trapping and manipulation of nanoparticles and study the plasmonic enhancement of fluorescence of a single fluorophore.

CPP 13.13 Mon 18:15 Poster B2

Preparation and physical characterization of magnetite nanoparticles (MNP) with Aminosilane shell — •Maryam Youhannayee[1], Stanislav Emelianov[1], Robert Rabenalt[2], and Mathias Getzlaff[1] — [1]Institute für angewandte physik, Heinrich-Heine-universität Düsseldorf — [2]Klinik für Urologie, Universitätsklinikum Düsseldorf

Magnetite Nanoparticles are widely studied because of their fascinating application and also biocompatibility and low toxicity in different fields of biology and medicine. These nanoparticles covered with Aminosilane are perfect candidates for hyperthermia therapy due to a nearly perfect prevention of wash-out. In this contribution, the synthesis of magnetite nanoparticles by chemical coprecipitation is presented. In a first step, magnetite nanoparticles were prepared by coprecipitation of ****2+ and ****3+ with ammonium. Subsequently, magnetite nanoparticles were coated with a ligand shell consisting of Aminosilane. Different techniques were used for morphology and structure characterization. Dynamic light scattering technique was carried out to investigate the size distribution of nanoparticles in wet environment. TEM images also prove the formation of spherical MNP. For characterizing the crystal structure, X-ray diffraction was used. These measurements show that different parameters such as preparation speed have a significant influence on the size of nanoparticles.

CPP 13.14 Mon 18:15 Poster B2

Hot Brownian Motion — •Alexander Fischer — Molecular Nanophotonics, Institut für Experimentalphysik I, Fakultät für Physik und Geowissenschaften, Universität Leipzig

Hot Brownian motion describes the motion of a heated microsphere in a liquid. A temperature field is created around the heated particle decaying with 1/r. The heat transferred from the particle to the surrounding fluid spreads around three orders of magnitude faster than the particle moves. Therefore a stationary temperature field is moving with the particle through the liquid. The non-equilibrium dynamics of the particle now differs from the unheated particles and an effective temperature and diffusion constant is introduced to describe the system. With the development of fast detection systems in the recent years and the possibility to restrict the motion of a microscopic object using an optical tweezer, an investigation of hot Brownian motion on short time scales has become possible. Due to the increasing impact of the particle's inertia and the surrounding fluid on short time scales, the motion of the particle is not completely random anymore. The aim of this research is to understand the fundamentals of an effective temperature definition for fluctuation dissipation relations under non-equilibrium conditions.

CPP 14: Poster: Polymer Networks and Elastomers, Hydrogels, Soft Robotics

Time: Monday 18:15–21:00 Location: Poster B2

CPP 14.1 Mon 18:15 Poster B2

Theoretical and experimental investigations of sealing systems — •Felix Senf and Othmar Marti — Institut für Experimentelle Physik, Ulm, Deutschland

In technical applications the sealing of hardware components is described with leakage rates based on different boundaries of the system. In general the physical rules state an absolutely sealed system is not possible. Different parameters like materials, surface structures, roughness parameters, closing forces and finally the design of the sealing system influence the function of the sealing joint. Engineer standards to describe the surface influence of sealing is only with roughness parameters of the hardware surface. They do not consider that roughness parameters are only statistical parameters with limited information to the real sealing behavior of the joint. Out of this 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 will 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 how sealing works.

CPP 14.2 Mon 18:15 Poster B2

Rheo-Raman: Chemo-mechanical monitoring of the cross-linking process in epoxy resins — •Moritz Strobel[1], Sabine Hild[1], Milan Kracalik[1], Carola Eyssell[2], and Bernhard Strauss[2] — [1]Johannes Kepler Universität Linz, Institute of polymer science, Altenbergerstraße 69, 4040 Linz, Austria — [2]voestalpine Stahl GmbH, voestalpine Straße 3, 4020 Linz, Austria

Mechanical properties of pure epoxy resins depend on the cross-linking density. Additives are used to tailor the properties of resins. To investigate their influence, two methods are used: A) Mechanical: Rheological data give information regarding the storage and loss modulus, viscosity, gel point etc. B) Chemical: Raman-microscopy is an excellent tool for the observation of cross-linking of epoxy resins, as it displays the splitting of the epoxy bonds at 1257 cm-1. The combination of both methods provides extensive insight in the curing process of different resin systems. By the in situ measurements of Raman and rheological data one can investigate the influence of the degree of cross-linking on the viscosity, storage and loss modulus. The simultaneous investigation of rheological and spectroscopic data enables a closer look at the processes and the responses of the system during the curing of resins. The Rheo-Raman-System consists of a Thermo Fischer DXR Raman Microscope and an Anton Paar MCR 502 Rheometer, linked by an optical adapter. The aim of the project is to investigate the cross-linking of epoxy resins with different additives like accelerators, flexibilizers or diluents, at different curing temperatures by in situ Rheo-Raman-measurements.

CPP 14.3 Mon 18:15 Poster B2

Replacement of organic solvents by using a soil-release polymer network — •Florian Szillat[1], Nacera Infed[1], Stephan Dietzel[2], Hans-Günter Hloch[1], and Jürgen Bohnen[1] — [1]wfk - Cleaning Technology Institute, D-47807 Krefeld, Deutschland — [2]Fogra - Forschungsgesellschaft Druck, D-81673 München

Printing machine housings are contaminated during sheet as well as web offset printing by deposition of aerosols (e.g. inkjet colour, moistening agents). These deposits induce printing errors due to carryover of inkjet colours on to be printed areas. We investigate sacrificial polymer network coatings that allow easy removal of adhesive inkjet colour after soaking with water. Further, this approach has the advantage of replacing organic solvents. To obtain a better understanding of their coating behaviour as well as their functionality during cleaning process surface tension, rheology as well as porosity are studied. Moreover, the polymer network's barrier effect is investigated via diffusion by means of finite difference method and scanning electron microscopy (EDX). The influence of polyetheramine composition with different molecular weight on the networks properties will be discussed and results of the practical use of such soil-release polymer networks will be shown.

CPP 14.4 Mon 18:15 Poster B2

Mechanical characterization of microcapsules and their rupture under compression — •Inga Melnyk[1], Ali Ghaemi[2], Alexandra Philipp[3], Andreas Bauer[4], Klaus Last[5], Stephan Gekle[2], and Andreas Fery[1] — [1]Institute Of Physical Chemsitry and Polymerphysics, Hohestr.6, 01069 Dresden, Germany — [2]Biofluid Simulation and Modeling, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth, Germany — [3]Physical Chemistry I, Universitätstr. 30, University of Bayreuth, Germany — [4]Henkel AG & Co. KG, Krefeld, Hentrichstr. 17-25, 47809 Krefeld — [5]Follmann GmbH & Co. KG, Heinrich Follmann-Str. 1, 32423 Minden

We present the characterization of the micromechanical properties of melamine microcapsules (MCs) on the single particle level by colloidal probe atomic force spectroscopy (CP-AFM).[1] The CP-AFM allowed for the precise measurement of the mechanical response of single capsules upon lateral linear elastic deformation in the small deformation regime (deformation << wall thickness). The obtained force-deformation curves were evaluated using contact mechanics model in combination with structural information by electron microscopy.[2] To study the rupture upon compression of MCs, higher forces were applied resulting in plastic deformation and ultimately in failure of the wall material. [3] We discuss the mechanical stability of the capsule material in the context the material requirements in various microcapsule applications. [1]*M. Pretzl et al. ACS Appl. Mater. Interfaces. 2012, 4, 2940*2948. [2]*M.P. Neubauer et al. Adv. Coll. Interface Sci. 2014, 207, 65*80. [3]*A.Ghaemi et al. Chem.Eng.Sci. 2015

CPP 14.5 Mon 18:15 Poster B2

Simulation of partially reversible networks under deformation or swelling — •Toni Müller[1,2], Jens-Uwe Sommer[1,2], and Michael Lang[1] — [1]Leibniz Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden, Germany — [2]Institute of Theoretical Physics, Technische Universität Dresden, Zellescher Weg 17, 01062 Dresden, Germany

Self-healing and partially reversible networks are interesting elastic materials that self-repair damage [1] and can be used to optimize energy dissipation [2]. Using the bond fluctuation model, we study networks made of varying fractions of reversible and irreversible bonds and investigate the molecular mechanism of bond breaking and rearrangement under uni-axial extension or swelling. One goal is to better understand the influences of the fracture energy and sticker density to optimize the properties of such materials.

[1] Long et al, Macromolecules 47, 7243 (2014).

[2] Sun et al. Nature 489, 133 (2012).

CPP 14.6 Mon 18:15 Poster B2

Microstructure analysis of PET via Raman spectroscopy and x-ray diffraction — •Birgit Neitzel, Florian Aschermayer, Milan Kracalik, and Sabine Hild — Johannes Kepler Universität Linz, Altenberger Str. 69, 4040 Linz Austria

Polyethylene terephthalate (PET) is a polymer applied in a broad field of applications requiring specific mechanical properties. For the tailoring of PET properties, its microstructure has to be controlled and characteristic parameters such as crystallinity and orientation of the polymer chains have to be investigated. In general, X-ray scattering is used, which has the disadvantage of recalculation data from an inverse room. In contrast, polarized Raman spectroscopy allows direct investigation of polymer micro-structure since for semi-crystalline polymers such as PET peaks can be assigned, which are only sensitive for chemical structure an do not change with polarization direction of incident light. Beside, also peaks can be found which change their intensity with polarization of the laser. These peaks can be used to determine the degree of crystallization (705 cm-1 and 998cm-1), as well as orientation of polymer chains (705 cm-1 and 1616 cm-1) Raman imaging allow the determine local crystallinity- and orientation distributions on different positions on the sample. The aim of this study is to find a correlation of micro-structure and mechanical properties using X-ray as well as Raman microscopy. Therefore the micro structure of an amorphous and an isotropic crystallized PET, as well as PET stretched to different strain rates will be investigated.

CPP 14.7 Mon 18:15 Poster B2

Synthesis and characterization of expandable hydrogels for flexible electronics — •Robert Gerstmayr, Melanie Baumgartner, Siegfried Bauer, and Sabine Hild — Johannes Kepler Universität Linz, Altenberger Straße 69, 4040 Linz, Österreich

Hydrogels are aqueous microgels and have found their way in a considerable number of applications but often with the disadvantage of their poor mechanical properties. To apply such polymers for flexible electronics they should be transparent, easy to manufacture and expandable, beyond that they should be able to interact with the encapsulated electronics. Double crosslinked microgels (DX microgels) are shown to achieve these properties. hydrogels formed by linking together polymer networks show a unique structure-property relationship. The preparation of hydrogels made of purely biological and nontoxic precursors, is based on commonly used and cheap biopolymers like gelatine or chitosan. These hydrogels are reinforced by acrylate precursors. The produced materials are focused on acrylate polymers, because they are excellent for crosslinking via photopolymerization. Further, gels forming ionically and covalently crosslinked networks to improve stretchability, are produced. The structure and mechanical properties in the nanometre range are investigated by atomic force microscopy (AFM). Raman spectroscopy is complementary used to characterize the chemical structure and their changes in contact with water, salt solution or the encapsulated electronic. Information about wetting properties and adhesion are obtained by contact angle measurement.

CPP 15: Poster: Functional Polymer Hybrids

Time: Monday 18:15–21:00 Location: Poster B2

CPP 15.1 Mon 18:15 Poster B2

Nanostructured hybrid block copolymer electrolytes as a membrane for lithium-ion microbatteries — •Maximilian Kaeppel, Ezzeldin Metwalli, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Solid-state polymer electrolyte membranes are promising alternatives to liquid electrolytes for energy storage related applications. A key challenge is to achieve a highly ionic conductive membrane that maintains both, high-modulus and chemical stability. The structure and conductivity of hybrid polymer electrolyte membranes composed of polystyrene-block-polyethylene oxide diblock copolymer (PS-b-PEO), lithium salt and ionic liquid (IL) were investigated. The PEO crystallization during the solution-casting of thin solid-state membranes was observed. The PEO crystallization is inhibited by increasing the doping level of both Li ions and IL. The high-modulus PS domains of the nanostructured hybrid membranes offers mechanical stability, while both the Li-containing PEO and IL enable the requisite high ionic conductivity. An optimized functional morphology of the hybrid membrane is achieved by enabling highly interpenetration hard PS and soft PEO/IL domains. The conductivity enhancement correlation with the evolved morphologies is proved.

CPP 15.2 Mon 18:15 Poster B2

Morphology of block copolymer electrolytes for rechargeable lithium batteries — •Bernhard Springer, Ezzeldin Metwalli, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

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 alkali metal-ions. The morphology of polylauryl methacrylate-block-polymethacrylic acid (PLMA-b-PMAA) BC electrolyte with three different ionic block volume fractions 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-ions containing BC hybrid films were examined for different morphologies using impedance spectroscopy.

CPP 15.3 Mon 18:15 Poster B2

Hybrid Based Thermoelectrica — •Anjani Kumar Maurya, Nitin Saxena, and Peter Müller- Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

High-efficiency thermoelectric (TE) materials are an important materials system for power generation that can directly convert thermal waste heat into electrical energy which plays a key role in our current challenge to develop alternative energy technologies to reduce our dependence on fossil fuels and to reduce greenhouse gas emissions. The power conversion efficiency of TE materials for TE generators is proportional to the so-called figure of merit ZT. Organic materials, such as polymers, are attractive thermoelectrics due to their low thermal conductivity, but face similar challenges in optimization as their inorganic counterparts. Inorganic hybrid composites, present a unique opportunity to optimize ZT via molecular and interfacial design in ways not possible in more classical systems. We investigate novel organic-inorganic hybrid materials for thermoelectric applications. The goal is to realize efficient low temperature ($T < 100°C$) thermoelectric hybrid thin films. We attempt to improve the figure of merit ZT, by combining nanostructured inorganic materials with the electrically conducting polymer blend PEDOT:PSS.

CPP 15.4 Mon 18:15 Poster B2

Polymer metal composite: direct patterning by E-beam lithography — •Parisa Bakhtiarpour[1], Annina Steinbach[2], Stefan Jenisch[2], Steffen Strehle[2], Othmar Marti[1], and Masoud Amirkhani[1] — [1]Institute of Experimental Physics, University of Ulm, 89069 Ulm, Germany — [2]Institute of Electron Devices and Circuits, University of Ulm, 89069 Ulm, Germany

Ionic polymer metal composites (IPMCs) have a wide range of applications as artificial muscle in robotic and micro robotics. To metalize ionic polymers such as Nafion, chemical reduction and electroless plating are common methods, but without the possibility to control the metal penetration into the polymer. The modality and depth of penetration have an important role in IPMC function, especially in micrometer sample size. To study the position and geometry of metal layer and their effect on performance, using a manageable method for metal electrodes fabrication is essential. In this work, E-beam has been used to pattern the polymer surface in desired shape with high value of accuracy and control. Physical methods like coating and sputtering can be applied after pattern process to cover the electrode area. We investigate various parameters for pattern formation and stable coating.

CPP 15.5 Mon 18:15 Poster B2

Template-assisted self-assembly of anisotropic plasmonic nanocuboids employing wrinkle-structured substrates — •Patrick T. Probst[1], Moritz Tebbe[2], Tobias A. F. König[1], and Andreas Fery[1] — [1]Institute of Physical Chemistry and Polymer Physics, Leibniz Institute of Polymer Research (IPF), Hohe Str. 6, Dresden, Germany — [2]Dept. of Physical Chemistry II, University of Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany

Tailored inter-particle coupling and substrate-supported plasmonic coupling effects are a prerequisite to generate electric and magnetic modes in colloidal optical metamaterials. Wrinkle-assisted self-assembly allows for the cost-effective construction of linear plasmonic arrays on macroscopic areas.[*Soft Matter* **2007**, *3*, 1530; *Farad. Discuss.* **2015**, *181*, 243] By multi-printing and selective transfer of assembled particle lines of defined morphology and periodicity, more complex structures are feasible.[*Langmuir* **2012**, *28*, 16745] Line spacing is determined by the template, whereas inter-particle spacing can be modified by a soft, polymeric spacer to tune the collective optical response. Thus, for the first time, we arrive at ensembles which show a clear signature of nanophotonic features in conventional UV/Vis/NIR spectroscopy homogenously over macroscopic areas, in accordance with electrodynamic simulations (GMMT, FDTD).[*Nano Lett.* **2014**, *14*, 6863] We present recent results in expansion of this assembly approach to anisotropic plasmonic nanocuboids and its perspectives toward metamaterial effects and concepts for light management.[*Mater. Today* **2014**, *18*, 185]

CPP 15.6 Mon 18:15 Poster B2

Mechanically tunable plasmon ruler by exploiting macroscopic colloidal line grating — •Anja Maria Steiner[1], Christoph Hanske[2], Tobias A.F. König[1], and Andreas Fery[1] — [1]Institute of Physical Chemistry and Polymer Physics, Leibniz Institute of Polymer Research (IPF), Hohe Str. 6, 01069 Dresden — [2]Dept. of Physical Chemistry 2, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth

Large-scale, template-assisted assemblies of plasmonic gold nanospheres[1] transferred to low-modulus, high-elongation elastomeric substrates (PDMS) represent a novel class of tunable optical systems. We present a tunable optical system with the ability to reversibly shift the plasmonic key resonance by mechanical deformation. This strain-dependent plasmonic response is observed with conventional UV/vis/NIR spectroscopy and is correlated to *in-situ* scanning probe microscoy measurements.

In strong agreement with finite-difference time-domain (FDTD) simulations the tunable optical response can be distinguished into two effects: First, the plasmonic resonance shift depending on the inter-particle distance within the lines (plasmon ruler). Second, the line-to-line coupling, which becomes dominant at a certain distance (grating effects).

Overall, controlling the optical response upon mechanical deformation gives the opportunity for mechano-optically active systems and soft optical sensors.

[1] Christoph Hanske *et al.*, Nano Lett., **2014**, 14, 6863-6871

CPP 15.7 Mon 18:15 Poster B2

Tailored Plasmonic Particle Arrays for Systematic Dark Field Spectroscopy — •Yannic Brasse[1], Tobias A. F. König[1], Matthias Karg[2], and Andreas Fery[1] — [1]Physical Chemistry and Polymer Physics, Leibniz Institute of Polymer Research (IPF), Hohe Str. 6, 01069 Dresden, Germany — [2]Physical Chemistry I, University of Bayreuth, Universitaetsstr. 30, 95440 Bayreuth, Germany

This work describes the fabrication of spaced plasmonic particle arrays for systematic dark field investigation. The major advantage of those substrates is the possibility of "high" throughput single particle spectroscopy in combination with the accessibility towards post-modifications. The concept is based on directed assembly of Poly(N-isopropylacrylamide) coated plasmonic colloids on micro contact printed polyelectrolyte multilayer films. Arrays of gold core particles were overgrown with gold and studied via dark field microscopy and spectroscopy. The presented method is highly suited for efficient screening of optical properties and catalytic reactions on the single particle level (M.B. Müller, ACS Nano, 2014, 8, 9410).

CPP 15.8 Mon 18:15 Poster B2

A Comparative Study of Photoinduced Deformation in Azobenzene Containing Polymer Films — •Sarah Loebner, Nataraja Sekhar Yadavalli, and Svetlana Santer — Institute of Physics and Astronomy, University of Potsdam, Germany

Here we report on light induced structuring and deformation of three photosensitive polymers differing in their glass transition temperature. To inscribe surface relief gratings, the polymer films were irradiated with interference pattern of different polarization: intensity interference pattern (IIP) and polarization interference pattern (PIP). The irradiation was conducted in-situ while simultaneously acquiring the topography change with AFM. The polymers show comparable kinetic of topography change and maximally attainable grating height under irradiation with IIP. The illumination with PIP results in larger grating height for all three polymers, but more pronounce topography change was found for the polymers of larger glass transition temperature.

We have also performed experiments where a rectangular piece of polymer film was cut out of the film using AFM lithography and irradiated with homogeneous light of linear polarization. For all three polymers we have found that the rectangular piece elongates along the electrical field vector and contracts in perpendicular direction.

CPP 16: High Efficiency Photovoltaics (joint session AKE/CPP, organized by AKE)

Time: Tuesday 9:30–10:30 Location: H3

Invited Talk CPP 16.1 Tue 9:30 H3

Multi junction concepts for photovoltaics and artificial photosynthesis: Critical points of current and future high-performance solar energy conversion — •Thomas Hannappel — Technische Universität Ilmenau, Department of Physics, Ilmenau, Germany

By far the highest solar energy conversion efficiencies have been achieved so far, when employing III-V-based semiconductor layer structures in multi junction approaches for optimum exploitation of the solar spectrum [1-3]. In these record-breaking multi-layer structures, interfaces are the most crucial parts in different regards. In devices for direct water splitting the solid-liquid interface is in particular delicate towards (photo)electrochemical corrosion and charge transfer. An interface with low-defect density between silicon and III-V compounds would be a major breakthrough and would not only add to solar energy conversion, but all kinds of opto-electronic devices.

To accelerate progress in these fields, it is essential to gain an atomic-scale understanding of critical and essential heterojunction preparation, including the complex physico-chemical processes and interface formations [4,5]. Here, we will present original analysis to scrutinise state-of-the-art preparation and to develop future solar energy conversion routes with multi junction concepts.

[1] M.M. May et al., Nat. Commun. 6 (2015) 8286 [2] A. Nakamura et al. Appl. Phys. Express 8 (2015) 107101 [3] F. Dimroth et al., Prog. Photovoltaics 22 (2014) 277 [4] O. Supplie et al., J. Phys. Chem. Lett 6 (2015) 464 [5] M.M. May et al., J. Phys. Chem. C. 118 (2014) 19032

Topical Talk CPP 16.2 Tue 10:00 H3

Monolithic perovskite/silicon-heterojunction tandem solar cells processed at low temperature — •Steve Albrecht[1], M. Saliba[2], J.P. Correa Baena[2], F. Lang[1], L. Korte[1], R. Schlatmann[1], M. K. Nazeeruddin[2], A. Hagfeldt[2], M. Grätzel[2], and B. Rech[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium-Photovoltaik, Kekuléstraße 5, 12489 Berlin, Germany — [2]Laboratory for Photonics Swiss Federal Institute of Technology (EPFL), Station 6, Lausanne, CH 1015, Switzerland

Tandem solar cells combining silicon and perovskite absorbers have the potential to outperform state-of-the-art high efficiency silicon single junction devices. However, the practical fabrication of monolithic silicon/perovskite tandem solar cells is challenging as material properties and processing requirements restrict the device design. We achieve a tandem cell efficiency of 19.9% with an open circuit voltage of 1.78 V for the reverse scan direction with a stabilized power output of 18.1% which is one the highest reported values to date. The monolithic integration was realized via low temperature processing of the semitransparent perovskite sub-cell. The tandem cell design is currently limited by the photocurrent generated in the silicon bottom cell that is reduced due to reflectance losses. Based on optical modelling and first experiments, we show that these losses can be significantly reduced by combining optical optimization including light trapping approaches. Therefore, this study highlights the great potential of monolithic silicon heterojunction/perovskite tandem solar cells.

CPP 17: Polyelectrolytes

Time: Tuesday 9:30–12:30 Location: H40

Invited Talk CPP 17.1 Tue 9:30 H40

Molecular Dynamics Simulations of Compacted Polyelectrolyte Complexes — •Diddo Diddens, Jörg Baschnagel, and Albert Johner — Institut Charles Sadron, Université de Strasbourg, CNRS UPR22, 23 Rue du Loess, 67034 Strasbourg Cedex 2, France

Compacted polyelectrolyte complexes (CoPECs) are gel-like materials created by ultracentrifugation [1] or extrusion [2] from solution-precipitated polyelectrolyte complexes. Usually, polyelectrolyte complexes have an ill-defined microscopic structure due to the fast aggregation kinetics of polyanions and polycations, which prevents the formation of an optimized ion pairing between positive and negative charges. Here, the two experimental strategies mentioned above offer a novel route to densify/reshape the complexes, which is difficult to achieve otherwise. However, although it is known from micrograph imaging that the CoPECs are highly porous, the precise effect of the centrifugation/extrusion on the polymer matrix is less clear.

We address this issue by mimicking the experimental centrifugation protocol in a fully atomistic Molecular Dynamics simulation. In particular, we identify the structural and dynamical changes during the individual stages of the compaction, which includes sedimentation, subsequent compression at the boundary and the behavior after centrifugation. These findings are discussed in context with the experimental observations.

[1] Porcel, Schlenoff, *Biomacromolecules*, **2009**, 10, 2968

[2] Shamoun, Reisch, Schlenoff, *Adv. Funct. Mater.*, **2012**, 22, 1923

CPP 17.2 Tue 10:00 H40

Long-ranged steric forces between physisorbed polyethylenimine-iron complexes — •Heba S. Mohamad, Heiko Ahrens, and Christiane A. Helm — Inst. for Physics, Uni Greifswald, 17487 Greifswald, Germany

The conformation of branched polyethylenimine (PEI) layers physisorbed from 1 mM Fe_2SO_4 solution is determined by force measurements. The colloidal probe technique (CPT) is used. PEI adsorbs flatly as purely electrostatic forces indicate. Additon of EDTA to the adsorption solution leads in pure water to steric forces as predicted for neutral grafted brushes. On addition of NaCl to the solution, the grafting density remains constant, yet the brush thickness shrinks and swells reversibly with the NaCl concentration.

X-ray reflectivity demonstrates that iron(II) is incorporated in the adsorbed polyethylenimine-iron complexes. Iron(ii) can be washed from the adsorbed complex without removing the PEI. Adsorption of gold nanoparticles (AuNP) onto a PEI layer with chains protruding into solution leads to an increased AuNP coverage compared to flat positvely charged surfaces.

CPP 17.3 Tue 10:15 H40

Polyelectrolyte complex nanoparticles: Adhesive material for local delivery of drugs and proteins — •Martin Müller[1,2], David Vehlow[1,2], Richard Petzold[1,2], Beatrice Woltmann[3], Diana Wehrum[3], and Ute Hempel[3] — [1]Leibniz-Institut für Polymerforschung Dresden e.V. — [2]Technische Universität Dresden, Chemie und Lebensmittelchemie — [3]Technische Universität Dresden, Physiologische Chemie

Mixing aqueous solutions of oppositely charged biorelated polyelectrolytes (PEL) in the presence of ionic compounds results in colloid dispersions of PEL complex (PEC) nanoparticles (NP) [1], which have potential for drug and protein delivery [2,3,4]. Casting these loaded PEC NP dispersions onto material surfaces results in coatings, from which drugs and proteins can be released into relevant aqueous media under local and kinetic control. Charged drugs like antibiotics and bisphosphonates and proteinogenic growth factors relevant for bone healing were loaded. Herein results on the adhesiveness and release kinetics of drug loaded PEC NP coatings under variation of drug/polycation/polyanion composition using in-situ-ATR-FTIR-, UV/VIS- and circular dichroism spectroscopy and SFM are presented [2,3,4]. Furthermore, results on the cytocompatibility of PEC NP coatings with respect to bone cells under variation of composition and net charge sign are given [4,5]. This work is sponsored by DFG (Transregio 79, Project M7). [1] Adv. Polym. Sci. 2014, 256, 197. [2] J. Pharm. Biomed. Anal. 2012, 66, 183. [3] Biointerphases 2013, 8, 25. [4] Biointerphases 2015, 10(1), 011001. [5] Int. J. Nanomedicine 2014, 9, 2205.

CPP 17.4 Tue 10:30 H40

Effect of Binary Polymer Mixtures on the Growth of Polyelectrolyte Multilayers (PEMs) — •Malte Passvogel[1], Peter Nestler[1], Ralf Köhler[2], Olaf Soltwedel[3], and Christiane A. Helm[1] — [1]Inst. for Physics, Uni Greifswald, 17487 Greifswald, Germany — [2]Helmholtz-Zentrum Berlin, 14109 Berlin, Germany — [3]MPI for Solid State Research, Outstation at FRM-II, 85747 Garching, Germany

Non-linear growth regimes of electrostatically assembled PEMs are investigated with in-situ ellipsometry. Poly(styrene sulfonate) (PSS) and poly(diallylmethylammonium) (PDADMA) are used (c_{NaCl} = 0.1 mol/L). Always, linear growth is preceded by a parabolic growth regime. For films of binary PDADMA mixtures, the composition in the film appears to be the same as in the adsorption solution. If PSS molecular weight (M_w) is below a threshold, 25 kDa, film build-up starts with an exponential growth regime, and pronounced PSS interdiffusion is found with neutron reflectivity using deuterated PSSd. 0.5 mol % PSS with high M_w in the adsorption solution prevents exponential growth. Neutron reflectivity shows no vertical center of mass movement of PSS with M_w above the threshold, both in the parabolic and the linear growth regimes. We suggest that polyelectrolytes (PEs) with high M_w adsorb with trains, tails and loops, while PEs with M_w below the threshold adsorb with one train and one tail only.

CPP 17.5 Tue 10:45 H40

Polyelectrolyte Multilayers – A Coarse-Grained Simulation Approach — Diddo Diddens[1], Martin Vögele[2], Andreas Heuer[1], Christian Holm[3], and •Jens Smiatek[3] — [1]Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster — [2]Max-Planck-Institut für Biophysik, Max-von-Laue-Straße 3, 60438 Frankfurt am Main — [3]Institute for Computational Physics, University of Stuttgart, Allmandring 3, 70569 Stuttgart

Polyelectrolyte multilayers are thin films created by the alternate adsorption of polyanions and polycations on a charged substrate. Due to the controlled layer-by-layer assembly, these materials offer a wealth to create tailored materials such as surface coatings or membranes. However, the detailed molecular structure in these films is difficult to probe by experimental techniques, whereas atomistic simulations, which are in principle able to capture the full microscopic details, are currently too demanding to study the layer-by-layer assembly beyond the first few adsorption steps [1].

To bridge this gap, we employ simulations of the coarse-grained MARTINI model, which has recently been adapted to poly(styrene sulfonate) (PSS) and poly(diallyl dimethyl ammonium) (PDADMA). A clear advantage of this model is that it – in contrast to very generic polyelectrolyte models – still retains the relevant chemical details. We mimic the layer-by-layer assembly in our simulations, and discuss the results in context with experimental data.

[1] Micciulla *et al.*, *Soft Materials*, **2014**, 12, S14

15 min. break

CPP 17.6 Tue 11:15 H40

Mutual effects in the temperature responsive behaviour of brush/multilayer composites — •Samantha Micciulla[1], Olaf Soltwedel[2], Oliver Löhmann[1], and Regine von Klitzing[1] — [1]TU Berlin, Germany — [2]FRM-II, MLZ Garching, Germany

The extensive use of polymers to prepare smart coatings is reasoned by their versatility to be assembled or synthesized in different geometries and to the large variety of responsiveness obtained by the choice of specific functionality. The present study focuses on the investigation of the temperature-responsive behavior of a composite made by polyelectrolyte multilayers (PEMs) physisorbed onto temperature-sensitive brushes. Ellipsometry was used to monitor the brush collapse from the thickness decrease as a function of temperature, while neutron reflectometry was applied to deduce the change of monomer distribution perpendicular to the substrate at temperatures below, across and above the phase transition, respectively. The results showed that the adsorption of PEMs enhanced the hydrophobicity of the charged region of the polymer brush, which directly interacts with the adsorbing chains, and this caused a shift of its phase transition to lower temperature. Moreover, the internal contrast obtained by combining hydrogenated brushes with deuterated PEMs allowed to highlight the penetration of polyelectrolyte chains inside the charged brush by comparing the neutron scattering length density profile of pure and corresponding PEM-capped brushes. This study demonstrates the possibility of creating complex brush/multilayer composites preserving the responsive behavior behind the significant interpolyelectrolyte interactions.

CPP 17.7 Tue 11:30 H40

Uptake and Spatial Distribution of Thiol-Capped Gold Nanoparticles in Strong Polyelectrolyte Brushes — •Dikran Kesal, Stephanie Christau, Patrick Krause, Tim Möller, and Regine von Klitzing — TU-Berlin, Straße des 17.Juni 124, 10623 Berlin, Germany

Polymer brushes are suitable candidates for the design of responsive smart surfaces which can be prepared by end-grafting polymers with the desired chain functionality on solid substrates. These surfaces have the ability to respond to external stimuli by changing their chemical or physical properties and can be used as a matrix for the immobilization of gold nanoparticles (AuNPs), which induce optical properties due to their surface plasmon resonance. In order to use the Brush/AuNP hybrids as smart surfaces, we must be able to control the arrangement of the NPs inside the brush and to correlate it with the optical properties of the composite system.

The present study addresses the distribution and uptake of charge switchable AuNPs inside poly-[2-(Methacryloyloxy) ethyl] trimethylammonium chloride (PMETAC) which yields a strong positively charged polyelectrolyte brush. The 5 nm AuNPs are capped with mercaptopropionic acid and are either negatively or uncharged depending on the pH. While some recent efforts have been made in terms of particle uptake and distribution in neutral (PNIPAM) and weakly charged (PDMAEMA) polymers by changing the thickness of the brushes and particle size, here the focus is on understanding how charges affect particle loading and penetration into the brush.

CPP 17.8 Tue 11:45 H40

Steady-state shear motion of polyelectrolyte-brush bilayers with oppositely charged polyelectrolyte stars — •Majid Farzin[1,2], Torsten Kreer[1], and Jens-Uwe Sommer[1,2] — [1]Leibniz Institute of Polymer Research Dresden Germany — [2]Institute of Theoretical Physics, Department of Mathematics and Natural Sciences, Technical University of Dresden Germany

Molecular dynamics simulations are employed to study polyelectrolyte-brush bilayers (PEB) with embedded polyelectrolyte stars (PES) under steady-state shear motion of two grafting surfaces. We use the Ewald-summation method to incorporate electrostatic interactions and the dissipative-particle-dynamics thermostat to account for hydrodynamic correlations. To study the influence of electrostatic interactions, we vary both the Bjerrum length and the fraction of charged brush monomers. Increasing the strength of electrostatic interactions leads to a slightly smaller osmotic pressure concomitant with a larger shear stress. Consequently, the resulting kinetic friction coefficient increases upon increasing of Bjerrum length or charge density. We relate this result to conformational properties, such as the distribution of stars within the bilayer, which depend strongly on the electrostatic interactions. Our study provides a significant advance towards a more realistic modeling of biological transport processes as they have previously preformed for electrically inert brushes of PEB without inclusions.

CPP 17.9 Tue 12:00 H40

Modified Dendrimers for drug delivery - a charge and size investigation — Brigitte Wiesner, Dietmar Appelhans, and •Ulrich Scheler — Leibniz-Institut für Polymerforschung Dresden e.V.

Dendrimers are frequently used as drug carriers. The high charge density makes them an ideal candidate for electrostatic binding. A combination of diffusion and electrophoresis NMR has been applied to study the effective size and charge of dendrimers and aggregates. The additional chemical information form chemical-shift resolution is used to differentiate dendrimers from small ligands bound. Thus the electrostatic interaction between PAMAM dendrimers and poly(styrene sulfonate) has been investigated as a function of pH. Functionalization of dendrimers with sugars like maltose control the interaction with lipids and model membranes. The effective charge of the modified dendrimers over pH is monitored in E-NMR. At low pH, the highly charged state, the hydrodynamic is larger because of the enhanced interaction with water. Diffusion NMR shows, that strong binding to lipid vesicles is hindered by the modification with maltose.

CPP 17.10 Tue 12:15 H40

The influence of transition metal cation size on protein phase behaviour — •Olga Matsarskaia[1], Michal Braun[1], Felix Roosen-Runge[2], Fajun Zhang[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]Institut Laue-Langevin, Grenoble, France

Transition metal cations induce many different types of interesting phase behaviour in aqueous solutions of negatively charged proteins, including reentrant condensation and liquid-liquid phase separation (LLPS) [1] which are involved in protein condensation diseases and may be used to optimise protein crystallisation [2]. We present a systematic study of the dependence of cation size on phase transitions in bovine serum albumin (BSA) using small-angle X-ray scattering (SAXS) and isothermal titration calorimetry (ITC). SAXS reveals an increase of the reduced second virial coefficient B_2/B_2^{HS}, i.e. a weaker interprotein attraction, with increasing cation size from Gd^{3+} to La^{3+}. This is consistent with a weaker LLPS with increasing cation size at room temperature and its eventual disappearance in the presence of La^{3+}. ITC shows cation-protein binding to be an entropy-driven process, presumably induced by the release of hydration water around the cations and surface residues of the protein. With decreasing cation size, the entropy-enthalpy balance of this reaction changes, as shown by both ITC and calculations [3], which has important implications for the understanding of the entropy balance of ions in solution.

[1] Zhang et al. (2014). PAC, 86, 191; [2] Sauter et al. (2015). JACS, 137, 1485; [3] Ciupka et al. (2010). PCCP, 12, 13215.

CPP 18: Molecular Electronics and Photonics

Time: Tuesday 9:30–12:45 Location: H42

CPP 18.1 Tue 9:30 H42

Coupled Electron-Nuclear Dynamics in Non-Adiabatic Processes — •Federica Agostini[1], Ali Abedi[2], Florian G. Eich[3], Neepa T. Maitra[4], Seung Kyu Min[5], Arne Scherrer[6], Axel Schild[1], Daniel Sebastiani[6], Yasumitsu Suzuki[7], Rodolphe Vuilleumier[8], and E. K. U. Gross[1] — [1]MPI of Microstructure Physics, Halle, Germany — [2]Universidad del País Vasco, San Sebastián, Spain — [3]MPI for the Structure und Dynamics of Matter, Hamburg, Germany — [4]CUNY, New York, USA — [5]UNIST, Ulsan, South Korea — [6]MLU Halle-Wittenberg, Halle, Germany — [7]University of Science, Tokyo, Japan — [8]UPMC, Paris, France

The Born-Oppenheimer (BO) approximation is widely employed to describe dynamical processes in molecular systems, based on the assumption that the typical time-scales of electronic and nuclear motion are adiabatically separable. This hypothesis allows to write the electron-nuclear wave function as a single product of an electronic eigenstate and a time-dependent nuclear wave function. Such an approximation, however, is not suited when non-adiabatic effects due the coupling between the nuclear motion and excited electronic states are important. The talk will show how the BO approximation can be made exact [PRL 105 (2010)], by preserving the single product form of the full wave function. This exact factorization approach will be introduced and used as a tool [PRL 110 (2013); JCP 142 (2015)] to interpret non-adiabatic processes. Algorithms will be derived [JCP 141 (2014); PRL 115 (2015); JCP 143 (2015)] to describe electronic non-adiabatic processes solving nuclear dynamics in terms of classical trajectories.

CPP 18.2 Tue 9:45 H42

Bending a chromophore in well-defined π-conjugated polygonic model systems: impact on photophysical properties — •Philipp Wilhelm[1], Thomas Stangl[1], Nina Schönfelder[2], Georgiy Poluektov[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

Conjugated polymers are a prime example for the complex interplay between morphology and function. Single-molecule spectroscopy has helped us in unraveling the large heterogeneity in this class of materials. But it has become apparent that even a single conjugated polymer chain contains such a complexity that it is difficult to derive a microscopic picture of the photophysical processes taking place in a single chain. We therefore introduce π-conjugated polygonic model systems, which all consist of a certain number of the same chromophoric unit. If we reduce this number the degree of bending increases, which makes the investigated molecules ideal candidates to study the impact of chromophore bending on spectroscopic observables. We go from the ensemble to the single molecule level to unmask the heterogeneity within the systems. By comparing the spectroscopic properties of molecules between different groups as well as the heterogeneity within a group, we can extract the influence of bending on the spectral properties. Extrapolating the results obtained from these systems onto conjugated polymers provides a highly heterogeneous picture regarding single chromophores that can exist on a conjugated polymer chain.

CPP 18.3 Tue 10:00 H42

Controlling position and orientation of molecules in a thin plastic film — •Felix Hofmann[1], Dominik Würsch[1], Vikas Aggarwal[2], Stefan-S. Jester[2], Jan Vogelsang[1], Sigurd Höger[2], and John Lupton[1] — [1]University of Regensburg, Regensburg, Germany — [2]University of Bonn, Bonn, Germany

For many single-molecule applications it is mandatory to embed the molecules under investigation in non-fluorescent host matrices. Single molecule spectroscopy was used to determine the position and orientation of molecules utilizing a monodisperse ring-shaped model system with a high triplet yield. The triplet state can be easily depopulated under ambient conditions for molecules close to the surface, but remains partly unquenched inside the film. Therefore, the fluorescence intensity serves as an observable for the spatial distribution of the molecules inside the film. The ring-shaped structure of the molecule together with excitation polarization spectroscopy reveals the orientation of the molecule with respect to the sample plane. A low modulation in intensity upon rotation of the polarisation of the laser indicates a molecule oriented flat with respect to the sample plane whereas a high modulation means that it is oriented perpendicularly to the sample plane. As an additional step in sample preparation, solvent vapor annealing enables diffusion of the molecules within the host matrix. This is achieved by applying a constant flow of solvent-saturated nitrogen to the sample, which lowers the glass transition temperature of the film. We found that after this additional treatment, all molecules lie flat with respect to the surface close to the plastic/air interface.

CPP 18.4 Tue 10:15 H42

Photon-correlation studies on single para-xylylene bridged perylene bisimide macrocycles — •Ulrich Müller[1], Peter Spenst[2], Matthias Stolte[2], Frank Würthner[2], and Jens Pflaum[1,3] — [1]Experimentelle Physik VI, Julius-Maximilians-Universität, Würzburg — [2]Institut für Organische Chemie, Julius-Maximilians-Universität, Würzburg — [3]ZAE Bayern, Würzburg

Future communication technologies demand for non-classical light sources based on efficient quantum emitters like organic molecules. The chemical variability and tunable fluorescence by proper substituents render Perylene Bisimides (PBIs) interesting candidates for implementation in single photon devices.

We will highlight the excitation dynamics of para-xylylene bridged PBI-macrocycles by means of photon-correlation measurements. These compounds show remarkable optical properties due to fast excitation energy transfer between the PBI entities [1]. We compare macrocycles with three and four chromophores with the PBI reference and show that the absorption cross section can be enhanced and the interaction with the surrounding matrix can be reduced while all macrocycles under study behave as single photon emitters. Utilizing the distribution of inter-photon delay times $g^{(2)}$ we determine the radiative transition rate $0.16(2)\mathrm{ns}^{-1}$ from the excited S1 to the ground state.

Our study advances the understanding of excitation and relaxation processes in multichromophoric systems and thus, promotes their application as single photon emitters.

[1] F. Schlosser et al., *Chem. Sci.* **3**, 2778 (2012)

CPP 18.5 Tue 10:30 H42

Ultrahigh time-resolutuion two-dimensional spectroscopy of polymer thin films — Antonietta De Sio[1,2], •Ephraim Sommer[1,2], Filippo Troiani[3], Julien Réhault[4], Margherita Maiuri[4], Giulio Cerullo[4], Elisa Molinari[3], and Christoph Lienau[1,2] — [1]Institut für Physik, Carl von Ossietzky Universität, 26197 Oldenburg, Germany — [2]Cernter of Interface Science, Carl von Ossietzky Universität, 26129 Oldenburg, Germany — [3]Instituto Nanoscienze - CNR, Centro S3, via Campi 213a, 41125 Modena, Italy — [4]IFN-CNR, Dipartimento di Fisica, Politecnico di Milano, 20133 Milano, Italy

Organic semiconductors have the remarkable property that their optical excitation not only generates charge-neutral electron-hole pairs (excitons) but also charge-separated polaron pairs with high yield. Although it is known that polaron pairs are formed on an ultrafast time scale, the microscopic mechanisms governing this formation are debated. We use two-dimensional optical spectroscopy to study this formation in a protoyptical polythiophene thin film with 10-fs time resolution. These spectra revealed multi-period oscillations with ~20 fs period, persisting for hundreds of femtoseconds, and peak splittings as signatures of persistent vibronic coherence at room temperature. Our data suggest that strong vibronic coupling causes polaron pair formation on a sub-20-fs time scale, accelerates charge separation dynamics and makes it insensitive against disorder-induced fluctuations of the vibronic levels.

CPP 18.6 Tue 10:45 H42

Electronic Properties of Optically Switchable Photochromic Diarylethene Molecules at Interface with Organic Semiconductors — •Qiankun Wang[1], Johannes Fisch[1], Björn Kobin[2], Stefan Hecht[2], and Norbert Koch[1] — [1]Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin, Brook-Taylor-Straße 6, 12489 Berlin, Germany — [2]Department of Chemistry, Humboldt-Universität zu Berlin, Brook-Taylor-Straße 2, 12489 Berlin, Germany

Photochromic organic molecules have attracted increasing interest for the development of low-cost multifunctional devices. Diarylethene (DAE) molecules, which are among the most interesting photochromes, show promising application potentials due to their high fatigue resistance and thermal bistability, and the interface energetics of DAE-based (bulk and planar) heterojunction is of high importance for understanding the effects on charge transport in photoswitchable devices. Here, the valence electronic structure upon switching of a photochromic diarylethene derivative, 1,2-bis (2-methyl-5-p-tolylthiophen-3-yl) cyclopent- 1-ene (DAE1) was measured by ultraviolet photoelectron spectroscopy. Switching between open and closed forms was followed in situ upon appropriate illumination with ultraviolet and visible light, respectively. The energy level alignment at interfaces between DAE1 and organic hole (electron) transport materials was observed to be affected by the photoisomerization process, which resulted in different charge transport energy barriers for holes (electrons) before and after light irradiation. Our experimental findings provide a rationale for photo-control of charge transport in organic electronic devices.

15 min. break

CPP 18.7 Tue 11:15 H42

Organic heterojunctions: Contact-induced molecular reorientation, interface states, and charge re-distribution — •Andreas Opitz[1], Andreas Wilke[1], Patrick Amsalem[1], Ulrich Hörmann[2], Ellen Moons[3], and Norbert Koch[1,4] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Institute of Physics, University of Augsburg, Augsburg, Germany — [3]Department of Engineering and Physics, Karlstad University, Karlstad, Sweden — [4]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

The planar heterojunction formed between the hydrogen and fluorine terminated copper phthalocyanines has been found to behave as charge generation layer [1]. Therefore, this interface was investigated by ultraviolet photoelectron and X-ray absorption spectroscopy. Pinning at the Fermi level of the underlying electrode is observed for both materials—one p type and the other one n type. This results in a sheet charge density at the organic/organic interface due to interfacial charge transfer. An interlayer with co-facial intermolecular arrangement, which differs from the respective bulk structures, at the interface was found by both spectroscopy techniques; this interlayer, noteworthy, is unpinned.

[1] A. Opitz et al., *Org. Electron.* **10** (2009) 1259–1267.

CPP 18.8 Tue 11:30 H42

Activation of Organometallic Dimers as n-Dopants for a Low Electron Affinity Organic Semiconductor — •Berthold Wegner[1], Xin Lin[2], Karttikay Moudgil[3], Stephen Barlow[3], Seth R. Marder[3], Antoine Kahn[2], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Germany — [2]Princeton University, USA — [3]Georgia Institute of Technology, USA

In the past years, several methods were developed to n-dope organic semiconducting materials in order to increase their conductivities. So far, however, these methods were only able to n-dope organic materials with electron affinities (EAs) as low as 4.0 eV. Recently, Guo et al. [1] introduced a new approach using organometallic dimers as air-stable precursors, with which they were able to n-dope several organic materials with EAs ranging down to 2.8 eV. In this work, we investigated the use of ultraviolet (UV) light to activate the n-doping of the low EA (2.4 eV) electron transport material phenyl-dipyrenylphosphine oxide ($POPy_2$) with two different organometallic dimers. Changes in the work function and conductivity of doped $POPy_2$ samples are measured for various doping concentrations using non-invasive contact potential difference and current-voltage measurements in the dark and in ultrahigh vacuum. Within only a few seconds of UV illumination, the conductivity was found to increase over several orders of magnitude and the Fermi level to be pinned at 2.6 eV. While both dimers show the same trends in their general doping behavior, they also differ in some details for which possible reasons are discussed.

[1] Guo et al. *Adv. Mater.* **24**, 699-703 (2012).

CPP 18.9 Tue 11:45 H42

Conduction mechanisms in polypyrrole (PPy)/pc-ZnO heterojunctions: role of the amount of FeCl3 as oxidizing agent — •Alejandra Castro-Carranza[1], Jairo C. Nolasco[2], Stephanie Bley[1], Florian Meierhofer[3], Lutz Mädler[3], Tobias Voss[4], and Jürgen Gutowski[1] — [1]Institute of Solid State Physics, Semiconductor Optics, University of Bremen, 28359 Bremen — [2]Energy and Semiconductor Research Laboratory, Carl von Ossietzky University of Oldenburg, 26129 Oldenburg. — [3]Foundation Institute of Material Science (IWT), Department of Production Engineering, University of Bremen, 28359 Bremen. — [4]Institute of Semiconductor Technology, TU Braunschweig University of Technology, 38092 Braunschweig.

The current-voltage characteristics of p-n hybrid heterojunctions based on polypyrrole (PPy) and polycrystalline ZnO (pc-ZnO) are analyzed by means of an electrical equivalent circuit. PPy is grown by oxidative chemical vapor deposition under three different amounts of FeCl3 used as oxidizing agent. The extracted parameters, together with the observed morphology of the PPy and the turn-on voltage values of the respective devices indicate that thermionic emission of holes occurs at the PPy/pc-ZnO heterojunction. For larger FeCl3 amounts used, an increment of recombination by tunneling of carriers occurs attributed to a narrowing of the depletion region due to an increment of traps states. These physical mechanisms are discussed on a schematic band diagram.

CPP 18.10 Tue 12:00 H42

The effect of intermolecular interaction on excited states in p-DTS(FBTTH2)2 — •Markus Reichenberger[1,2], John A. Love[3], Alexander Rudnick[1,2], Sergey Bagnich[1], Fabian Panzer[1,2], Anna Stradomska[4], Guillermo C. Bazan[3], Thuc-Quyen Nguyen[3], and Anna Köhler[1,2] — [1]Experimental Physics II — [2]Bayreuth Institute of Macromolecular Research (BIMF), University of Bayreuth, 95440 Bayreuth, Germany — [3]Center for Polymers and Organic Solids, Departments of Chemistry & Biochemistry and Materials, University of California, Santa Barbara, California 93106, United States — [4]School of Chemistry, University of Glasgow, Glasgow G12 8QQ, United Kingdom

Using optical spectroscopy in solution and thin film, and supported by quantum chemical calculations, we investigated the aggregation process of the donor-acceptor type molecule p-DTS(FBTTH2)2. We demonstrate that cooling a solution induces a disorder-order phase transition that proceeds in three stages analogous to the steps observed in semi-rigid conjugated polymers. By analyzing the spectra we are able to identify the spectral signature of monomer and aggregate in absorption and emission. From this we find that in films the fraction of aggregates is near 100 % which is in contrast to films made from semi-rigid conjugated polymers.

CPP 18.11 Tue 12:15 H42

Optical and structural properties of electrochemically prepared porphyrin thin films — •Kristina Lovrek[1,2], Karsten Hinrichs[2], Klaus Rademann[3], Felix Rösicke[1,4], and Jörg Rappich[4] — [1]Humboldt-Universität zu Berlin, School of Analytical Sciences Adlershof (SALSA), Unter den Linden 6, 10099 Berlin — [2]Leibnitz-Institut für Analytische Wissenschaften - ISAS - e.V., ISAS Berlin, Schwartzschildstrasse 8, 12489 Berlin — [3]Humboldt-Universität zu Berlin, Department of Chemistry, Brook-Taylor-Strasse 2, 12489 Berlin — [4]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH Inst. Silizium-Photovoltaik, Kekulèstasse. 5, D-12489 Berlin

Properties of thin porphyrin films on semiconductor surface for use in electronic devices are investigated. Thin porphyrin films were prepared via three different synthetic routes. Different optical techniques are used for investigation of their optical and structural properties. Atomic force microscopy, UV/vis and infrared in-situ ellipsometry are used to obtain information on their optical constants, layer thickness, interactions between molecules, mechanism of reaction and structural changes. Spectral information is obtained with IR reflection spectroscopy and IR ellipsometry. Vibrational bands are analyzed with respect to the chemistry and structure.

CPP 18.12 Tue 12:30 H42

Direct probe of injection efficiency in asymmetric coplanar organic transistors — •Karin Zojer[1], Thomas Rothländer[2], Herbert Gold[2], Anja Haase[2], and Barbara Stadlober[2] — [1]Institute of Solid State Physics and NAWI Graz, Graz University of Technology, Graz, Austria — [2]MATERIALS Institute for Surface Technologies and Photonics, JOANNEUM RESEARCH Forschungsgesellschaft mbH, 8160 Weiz, Austria

Injection of carriers from the metal contacts into organic semiconductors crucially determines the performance of organic electronic devices, as mobile charges must essentially be provided by the contact. Asymmetric coplanar transistors with overlaps or single-sided small gaps between source/drain and gate electrode allow us to locally modify the electric field solely near the injecting contact. Utilizing self-aligned nanoimprint lithography interlayer electrode offsets between -0.2-1.7 μm were realized. Given that injection typically occurs via Schottky-type barriers, the comparison of the operation of the same device with either source-sided gap or drain-sided gap directly probes the impact of the electric field on the injection efficiency without changing biases and injection barriers. We explain that transistors with a gap between source and gate electrode operate and that the profound reduction in current can be attributed to inhibited injection.

CPP 19: Microswimmers (joint session BP/CPP/DY, organized by DY)

Time: Tuesday 9:30–13:00 Location: H47

Invited Talk CPP 19.1 Tue 9:30 H47

Amoeboid swimming — •Chaouqi Misbah — CNRS and Univ. Grenoble, France

Microorganisms, such as bacteria, algae, or spermatozoa, are able to propel themselves forward thanks to flagella or cilia activity. By contrast, other organisms employ pronounced changes of the membrane shape to achieve propulsion, a prototypical example being the Eutreptiella gymnastica. Cells of the immune system as well as dictyostelium amoebas, traditionally believed to crawl on a substratum, can also swim in a similar way. We develop a model for these organisms. It is shown that fast propulsion can be achieved with adequate shape adaptations. We investigate the effect of confinement. A complex picture emerges. In particular it is found that optimal swimming can be obtaiend for a special confinement, and that the nature (pusher or puller) of the swimmer depends on confinement. The swimmer is often found to excecute ample excursion (navigation) in the channel.

CPP 19.2 Tue 10:00 H47

Meandering liquid crystal droplet swimmers — •Carsten Krüger, Corinna Maass, Christian Bahr, and Stephan Herminghaus — Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany

Liquid crystal microswimmers immersed in an aqueous surfactant solution at concentrations above the critical micelle concentration show self-propelled motion. The droplets dissolve into surfactant micelles [1], producing an inhomogeneous surfactant distribution in the continuum, propelling the droplets via Marangoni flows at the interface [2,3].

Below the nematic-isotropic transition we observe regular meandering trajectories, which change to a persistent random walk when the droplets are made isotropic by heating. This offers a unique possibility to tune the swimming behavior. We observe a distortion of the nematic director field, with the central defect pulled towards the droplet apex, but angled away from the direction of motion. This is consistent with a constant torque caused by a distortion of the defect pattern by the external and internal flow fields, acting against the elastic field associated with the nematic order. It also gives rise to the twofold symmetry break required for helical motion, as proposed by theory, e.g. in [4].

We use polarized microscopy to observe defect structures, PIV to image flow fields and are able to track freely moving droplets in 3D with a light sheet setup. [1] K. Peddireddy et al., Langmuir 28, 12426 (2012). [2] S. Herminghaus et al., Soft Matter 10, 7008 (2014). [3] C. C. Maass et al., Annu. Rev. Cond. Mat. 7, in press (2016). [4] H. Crenshaw, Amer. Zool. 36, 608 (1996).

CPP 19.3 Tue 10:15 H47

Dynamical density functional theory of microswimmers — •Andreas M. Menzel, Arnab Saha, Christian Hoell, and Hartmut Löwen — Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany

Microswimmers are found in nature in the form of self-propelling microorganisms, or they can be realized artificially, e.g. as Janus particles propelling due to self-induced phoretic effects. To describe and predict the collective behavior of many such interacting microswimmers on the mesoscopic level, statistical approaches are necessary.

Along these lines, we here report on a newly established dynamical density functional theory (DDFT). This theory includes steric as well as hydrodynamic interactions between individual swimmers within dilute and moderately concentrated suspensions of microswimmers. Minimal model microswimmers are considered. They self-propel by setting the surrounding fluid into motion, which leads to additional hydrodynamic interactions. Both pusher and puller swimming mechanisms are taken into account.

Via numerical simulations, our DDFT is demonstrated to reproduce effects recently observed in agent-based simulations. In a spherical trapping potential, this includes the formation of density rings and the self-organization in a symmetry-breaking state that resembles a hydrodynamic fluid pump. An additional instability is predicted that destabilizes the pumping state.

CPP 19.4 Tue 10:30 H47

Dynamics of a single self-propelled particle — •Christina Kurzthaler, Sebastian Leitmann, and Thomas Franosch — Department for Theoretical Physics, University of Innsbruck, Innsbruck, Austria

The dynamics of a single self-propelled particle in two dimensions is analyzed in terms of the intermediate scattering function, i.e. the characteristic function of the random displacements. Its analytical solution is derived by solving the Fourier transform of the Fokker-Planck equation which has the form of a complex Mathieu equation. Exact expressions for the mean-square displacement and non-Gaussian parameter are obtained as derivatives of the intermediate scattering function. For large wave numbers, oscillations in the intermediate scattering function reflect the persistent swimming motion, whereas at small wave numbers diffusive behavior emerges with an effective diffusion coefficient depending on the velocity and rotational diffusion of the swimmer.

CPP 19.5 Tue 10:45 H47

Droplet swimmers in complex geometries: Autochemotaxis and trapping at pillars. — •Chenyu Jin, Corinna Maass, Carsten Krüger, and Stephan Herminghaus — MPI for Dynamics and Self-Organization, 37077 Göttingen, Germany

Many organisms communicate by trail mediated signalling or autochemotaxis: their motion is influenced by their own emission of a chemical attractant or repellent, diffusing slowly compared to typical agent velocities. This causes gradient forces acting both on themselves as well as on other individuals. Meanwhile, geometrical confinement also influences the behaviour of microswimmers, e.g., pusher-type swimmers attach to curved interfaces depending on the interplay of hydrodynamic interaction and trajectorial persistence. It is of high biological relevance to have a well-controlled, tunable artificial model system exhibiting these traits.

A promising candidate are self-propelling liquid crystal droplets in an aqueous surfactant solution. They gain propulsion energy by micellar solubilisation, with filled micelles acting as a chemical repellent. We can tune the key parameters swimmer size, velocity and persistence length. We use microfluidic pillar arrays of variable radii to provide a convex wall to attract the swimmer, bend its trajectory and to force it to revert to its own trail. Hence, we investigate the interplay of wall attraction, persistence of motion, and negative auto-chemotaxis. We observe repulsion for highly curved surfaces, stable trapping at large pillars, and a narrow transition region, where negative autochemotaxis makes the swimmers detach after a single orbit.

15 min break

CPP 19.6 Tue 11:15 H47

Dimensionality matters in the collective behaviour of active emulsions — •Corinna Maass, Carsten Krüger, and Stephan Herminghaus — MPI for Dynamics and Self-Organization, 37077 Göttingen, Germany

Microswimmer systems like plankton constitute an important part of our ecosystem. The description of such systems is complex, as it involves large numbers of agents, long range hydrodynamic interactions and nontrivial boundary conditions like turbulent flows and complex interfaces. They exhibit rich and sometimes puzzling behaviour like the high species diversity referred to in the Plankton Paradox, or self organised bioconvection of gravitactic bacteria. This complexity makes them hard to treat analytically and numerically. Large scale simulations usually have dimensional restrictions or exclude hydrodynamic interactions, which has to be considered in comparisons with natural systems. Simple, tunable artificial swimmer systems can help bridging this gap.

Our experimental system consists of an active emulsion of self propelling liquid crystal droplets under variable microfluidic confinement and with tunable buoyancy. While changing the system's geometry from a quasi 2D confinement to a full 3D bulk reservoir, we observe a pronounced transition from only transient local aggregation over line formation to a large scale clustering phase stabilised by self-generated convection patterns. We studied this clustering behaviour in more detail with respect to reservoir height and buoyancy.

CPP 19.7 Tue 11:30 H47

Quantification of modular phoretic micro-swimmers — •Ran Niu, Christopher Wittenberg, Julian Weber, Denis Botin, and Thomas Palberg — Institut f. Physik, JGU Mainz, Staudingerweg 7, D-55128 Mainz, Germany

We have studied the swimming behavior of modular phoretic 2D micro-swimmers with particular focus on collective and cooperative effects[1,2]. These were exploited to proceed from isolated electrolyte releasing particles, driven by electro-osmotic flow field across a charged substrate, to multi-component complex, capable of self-generated, self-directed motion, transport and release of cargo and mutual long ranged interactions. Using optical techniques, such as microscopy and super-heterodyne laser doppler velocimetry, we accurately measured and characterized the swimmer properties and dynamics. From PH gradient measurements and particle tracking, we quantified the electric field and flow field around electrolyte releasing particle. The dependence of field strength on time and the size of electrolyte releasing particle were also determined. This provides the base for the quantitative understanding and establishing of a reliable model.

[1] T. Palberg, H. Schweinfurth,T. Koller,H. Muller,H.J. Schope, and A Reinmuller, European Physics Journal Special Topics 2013, 222:2835-2853. [2] A. Reinmuller, H.J. Schope, and T. Palberg, Langmuir 2013, 29:1738*1742.

CPP 19.8 Tue 11:45 H47

Confinement of Single Microswimmers in Circular Microfluidic Chambers — •Tanya Ostapenko, Thomas Böddeker, Christian Kreis, Fabian Schwarzendahl, Marco G. Mazza, and Oliver Bäumchen — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Fassberg 17, 37077 Göttingen, Germany

The characteristics of active fluids, such as suspensions of biological microswimmers, may not only originate from the mutual interactions between the constituents, but also from interactions with interfaces and confining walls. In fact, the natural habitats of many living organisms are complex geometric environments, rather than bulk situations. The influence of interfaces on the dynamics was recognized as an important factor, and there are differences in the way that pusher-type swimmers (e.g. *E. coli*) and puller-type swimmers (e.g. *C. reinhardtii*) behave close to flat interfaces. Using experiments and simulations, we report on the dynamics of single puller-type swimmers in 2D circular microfluidic chambers. We find that the radial probability distribution of trajectories displays a characteristic wall hugging effect, where swimmers remain trapped at a concave interface for decreasing chamber size. For trajectories in the vicinity of the concave wall, an alignment of the local swimming direction with the local wall tangent is observed. In contrast, the swimmers tend to scatter off convex interfaces with short interaction times. Based on geometric arguments involving the swimmer's persistence length, we explain this entrapment effect at concave interfaces.

CPP 19.9 Tue 12:00 H47

Tumbling of an E. coli: role of rotation-induced polymorphism and external shear — •Tapan Chandra Adhyapak and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, D - 10623 Berlin, Germany

Many multiflagellated bacteria such as E. coli adopt a run-and-tumble strategy to detect and direct themselves in chemical gradients in their surroundings. Tumbles are events which mark nearly abrupt changes in the direction of straight runs of the bacterium. Reversal of rotation of one or more of the flagella, which under normal rotation act as the propelling part of the bacterium, initiates these tumbles. Simultaneously, flagella that are reverse rotated are observed to undergo a series of polymorphic transitions between different flagellar states [1].

To understand the need, if there is any, of these transitions for an effective tumbling event has remained a long-standing problem. We present here a detailed numerical investigation unraveling the correlation between flagellar conformational changes and an efficient tumbling strategy for E. coli. Importance of these transitions in comparison to the contribution from hydrodynamic and steric interactions [2] will be addressed. At the end the nature of a tumbling event in sheared environment will also be discussed.

[1] R. Vogel and H. Stark, Phys. Rev. Lett. **110**, 158104 (2013).
[2] T.C. Adhyapak and H. Stark, Phys. Rev. E **92**, 052701 (2015).

CPP 19.10 Tue 12:15 H47

Sperm Cells in Structured Microchannels — •Sebastian Rode, Jens Elgeti, and Gerhard Gompper — Theoretical Soft Matter and Biophysics, Institute of Complex Systems (ICS-2) , Forschungszentrum Jülich, 52425 Jülich, Germany

At low Reynolds numbers and in confinement, the directed motion of a self-propelled microswimmer is strongly influenced by steric and hydrodynamic surface interactions [1-2]. Our mesoscale hydrodynamics simulation allow the study of various flagellated and ciliated microorganisms in this environment, ranging from a single flagellated sperm cell to multiciliated microswimmers. In particular, we have studied the motion of sperm in geometrically structured (zig-zag) microchannels. This is an interesting geometry for the manipulation and sorting of sperm cells. In general, sperm swim along the channel walls, but can be deflected from the wall at sharp bends. We found that the effective adhesion of a sperm cell to a curved surface depends both on the envelope of its sinusoidal beating shape and on the orientation of its beating plane. We present a heuristic argument explaining this dependence by an interplay of steric and hydrodynamic surface interactions. Our results are in qualitative agreement with recent microfluidic experiments and might provide a better insight in the mechanisms of sperm navigation under strong confinement.

[1] J. Elgeti et al., Rep. Prog. Phys. 78, 056601 (2015)
[2] J. Elgeti et al., Biophys. J. 99, 1018 (2010)

CPP 19.11 Tue 12:30 H47

Cross-stream transport of asymmetric particles driven by oscillating shear — •Matthias Laumann[1], Paul Bauknecht[2], Stephan Gekle[2], Diego Kienle[1], and Walter Zimmerman[1] — [1]Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Biofluid Simulation and Modeling, Universität Bayreuth, 95440 Bayreuth, Germany

We study the dynamics of asymmetric, deformable particles in oscillatory, linear shear flow. By simulating the motion of a dumbbell, a ring polymer, and a capsule we show that cross-stream migration occurs for asymmetric elastic particles even in linear shear flow if the shear rate varies in time. The migration is generic as it does not depend on the particle dimension. Importantly, the migration velocity and migration direction are robust to variations of the initial particle orientation, making our proposed scheme suitable for sorting applications of various elastic Janus-like particles.

CPP 19.12 Tue 12:45 H47

Calibration method for pH measurements with spatial and temporal resolution — •Julian Weber — Staudingerweg 7, 55128 Mainz

According to the framework of modular microswimmers, the field flow around involved particles is of great interest and can be measured by Doppler velocimetry. Here I present a special method for measuring the pH gradient around a cationic exchange resin. First gradient measurements are demonstrated.

CPP 20: Focus: Functional Polymer Hybrids I

Organizers: Marina Grenzer (Leibniz-Institut für Polymerforschung Dresden e.V.), Thomas Hellweg (Universität Bielefeld), Svetlana Santer (Universität Potsdam)

Functional polymer hybrids represent a combination of synthetic polymer with organic/inorganic additives which render material a new function. So, addition of iron particles provides the hybrid material with a strong sensitivity against magnetic fields. A vast research field includes polymers with light-sensitive moieties and plasmonic hybrids converting the light energy into heat. The session aims to bring together representatives from leading groups to discuss in a congenial atmosphere recent advances and new challenges in this exciting field.

Time: Tuesday 9:30–12:45 Location: H51

Invited Talk CPP 20.1 Tue 9:30 H51

Photoinduced Surface Patterning in Azo-Polymers: How Can Supramolecular Functionalization Strategies Serve Us? — •Arri Priimägi — Department of Chemistry and Bioengineering, Tampere University of Technology, Finland

The light-induced surface patterning in azobenzene-containing materials is a good example of the photomechanical power of azobenzene, the isomerization of which can actuate macroscopic motions into the material system it is incorporated into. The surface deformation can be very pronounced, and a great deal of research effort is being put into gaining fundamental understanding on the light-induced motions as well as into the use of the photoinduced surface patterns in applications in photonics and nanofabrication.

Supramolecular functionalization strategies, i.e., the use of non-covalent intermolecular interactions to attach azobenzenes into passive host matrices, are pertinent from both fundamental and applied perspectives. In particular, supramolecular interactions provide a platform to experimentally study the structure-function relationships that govern the surface patterning and the limits beyond which the process does not occur anymore. Even weak interactions make a large difference, and not only the strength but also the directionality of the noncovalent interaction must be considered when designing supramolecular materials that move efficiently in response to light.

CPP 20.2 Tue 10:00 H51

Cooperative Photo-Switching in Nanofibers of Azobenzene Oligomers — •Stefan Kowarik[1], Christopher Weber[1], Manuel Gensler[1], Tobias Liebig[1], Anton Zykov[1], Linus Pithan[1], Jürgen P. Rabe[1,3], Stefan Hecht[2,3], and David Bléger[2] — [1]Department of Physics & — [2]Department of Chemistry & — [3]IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

The integration of molecular switches into hierarchical assemblies makes it possible to amplify a single-molecule mechanical photoresponse to macro-scale events involving many molecules. Here, we demonstrate that multi-azobenzene oligomers can assemble to form robust supramolecular nanofibers in which they can be photo-switched repeatedly between the E- and Z-configuration. While in isolated oligomers the azobenzene units undergo reversible photoisomerization independently, in the nanofibers they are coupled via mechanical and electronic interactions and switch cooperatively as evidenced by unusual thermal and kinetic behavior. Depending on the fraction of Z-azobenzene in the nanofibers the photoisomerization rate from the Z-isomer to the E-isomer is increased by more than a factor of 4. This demonstrates the great potential of coupling individual photochromic units for increasing their quantum efficiency and amplifying molecular switching events with potential relevance for actuation and sensing.

CPP 20.3 Tue 10:15 H51

Optically controlled shape of soft nano-objects — •Selina Schimka[1,2] and Svetlana Santer[1] — [1]University of Potsdam, 14476 Potsdam, Germany — [2]Max Plank Institute of Colloids and Interfaces, 14424 Potsdam, Germany

What have acid-group containing microgels and DNA in common? Right, both of them are negatively charged polymers, drawing attention of research because of possible applications in biological and biomedical application.

But beside this, both are soft nano-objects, that can be reversibly and non-invasively changed in their shape by light, with assistance of an azobenzene containing agent [1,2]. Althought the mechanisms behind this process differs if microgel or DNA is used, and apparently even with the used azobenzene containing agent, the effect is quite similar - from a widely expanded state (swollen microgel or decompacted for DNA) with a high water content, they undergo a transition to a compacter, smaller state (shrunken microgel or compacted DNA), and back to the expanded state, depending on the illumination conditions. This behavior is in any case related to the trans cis isomerization of the azobenzene containing agent, which can be switched between a hydrophilic trans (visible light) and a hydrophobic cis (UV light) state, which alters its interaction with the microgel/DNA. Regarding previous works, we consider questions of toxicity and systematic behavior by the help of a set of new azobenzene containing agents.

[1] A.L.M. Le Ny, *JACS* **2006**, 128, 6400.

[2] Y. Zakrevskyy, *Adv Funct Mater* **2012**, 22, 5000.

CPP 20.4 Tue 10:30 H51

Photoisomerization kinetics in azobenzene-containing polymers — •Tatiana Petrova[1,2], Jaroslav Ilnytskyi[1,3], Vladimir Toshchevikov[1], and Marina Saphiannikova[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V. — [2]Cherepovets State University, Russia — [3]Institute for Condensed Matter Physics, Lviv, Ukraine

Azobenzene-containing polymers belong to a class of smart materials, which are able to transform the light energy into mechanical stress [1, 2]. We study the photoisomerization kinetics in azobenzene-containing polymers using the coarse-grained simulations and a theoretical model for the kinetic processes. The reorientation of azobenzene chromophores under trans-cis and cis-trans isomerization processes are taken explicitly into account. It is shown that the population kinetics of trans- and cis-isomers and their stationary orientation states depend on the ratio between characteristic times which characterize the rotation diffusion of the isomers, the frequency of photoisomerization of trans-isomers and the time of cis-trans relaxation. The form of the reorientation potential of the mean force acting on the isomers is analyzed and its use is validated.

[1] T. Petrova et al. Soft Matter 11 (2015) 3412

[2] J. Ilnytskyi et al. ChemPhysChem 16 (2015) 3180

CPP 20.5 Tue 10:45 H51

Approach to macroscopic functional colloidal optical metamaterials — •Tobias A.F. König[1], Svetlana Santer[2], and Andreas Fery[1] — [1]Institute of Physical Chemistry and Polymer Physics, Leibniz Institute of Polymer Research (IPF), Dresden — [2]2Department of Experimental Physics, Potsdam

We are interested in optical and mechanical interactions between functionalized nanoparticles and functionalized surfaces to assemble nanoparticles on the macroscopic area. Two assembly approaches will be discussed in this contribution: First, using the prevailing surfaces forces to move nanoobjects and second, using lithography free templates to assemble plasmonic nanoparticles. In the first approach, we use a plasmonically induced azobenze mass transport to move nanoparticles. This allows us to analyse the underlying plasmonic effects by changing polarization or wavelength observed at a fixed position. In the second approach, we present ensembles of surface-ordered nanoparticle arrangements, which are formed by template assisted self-assembly of monodisperse, functionalized gold nanoparticles in wrinkle-templates. Both methods are confirmed with electromagnetic simulations (FDTD) to analyse the responsible forces of the nanoimprints and to discuss the collective optical response of the assembled nanoparticles. We discuss the expansion of these approaches towards colloidal optical metamaterials and light management concepts.

15 min. break

Invited Talk CPP 20.6 Tue 11:15 H51

Plasmon coupling in self-assembled colloidal monolayers — •Matthias Karg — Physical Chemistry I, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth, Germany

Organized nanoscale structures which can guide or manipulate the propagation of electromagnetic fields at optical frequencies are of great importance for applications in sensing, all-optical computing and photovoltaics. While such structures are typically created by lithographic approaches, the realization of optically functional superstructures through bottom-up assembly of colloidal building blocks remains challenging. In this contribution I will report on our latest results of using wet-chemically synthesized plasmonic colloids, their assembly into highly periodic superstructures as well as their optical performance. Structural control is achieved by using polymer encapsulation strategies which allow us to tune inter-particle interactions[1]. Different methods for 2D assembly will be presented yielding isotropic as well as anisotropic particle arrays of high order[2]. Long-range dipolar plasmon resonance coupling is observed for assemblies with extraordinarily high degrees of order[3]. The enhanced Q-factors of these coupled arrays are promising for low-threshold plasmonic lasing.

[1] A. Rauh, T. Honold, M. Karg, Colloid Polym Sci 2015, DOI: 10.1007/s00396-015-3782-6 [2] T. Honold, K. Volk, A. Rauh, J.P.S. Fitzgerald, M. Karg, J. Mater. Chem. C 2015, 3, 11449-11457 [3] K. Volk, J.P.S. Fitzgerald, M. Retsch, M. Karg, Adv. Mater. 2015, DOI: 10.1002/adma.201503672

CPP 20.7 Tue 11:45 H51

Thermoelectric thin films based on a polymer/nanoparticle nanocomposite — •Nitin Saxena[1,2], Anton Greppmair[3], Mihael Coric[4], Jan Wernecke[5], Stefanie Langner[5], Michael Krumrey[5], Eva M. Herzig[4], Martin S. Brandt[3], and Peter Müller-Buschbaum[1,2] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Center for NanoScience, LMU München, 80539 München, Germany — [3]TU München, Walter-Schottky-Institut and Physik-Department, 85748 Garching, Germany — [4]TU München, Munich School of Engineering, 85748 Garching, Germany — [5]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 the large-scale application of thermoelectrics. In order to overcome these limitations, we pursue a hybrid approach combining the semiconducting polymer blend PEDOT:PSS for its high electrical conductivity and inorganic nanoparticles in order to reduce thermal conductivity within the thin film. We investigate the influence of the nanoparticles on the morphology by GISAXS and correlate this with changes in the thermoelectric behavior. In addition, we also investigate the thermal conductivity of pristine PEDOT:PSS and of the hybrid film by IR thermography, in order to ultimately calculate the figure-of-merit ZT.

CPP 20.8 Tue 12:00 H51

Mesoscopic modeling of magnetic gels: reversibly switching elastic and superelastic stress-strain properties — Peet Cremer, Giorgio Pessot, Hartmut Löwen, and •Andreas M. Menzel — Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany

Magnetic gels are generated by embedding magnetic colloidal particles into a permanently crosslinked, possibly swollen elastic polymer matrix. Several of their material properties can be reversibly switched from outside by applying external magnetic fields during operation. We model the switchability of such material properties on the mesoscopic level.

Previously, we had introduced simplified dipole-spring approaches to study the reversible tunability of linear elastic and dynamic properties. In contrast to that, we here mainly report on switchable nonlinear stress-strain properties. For this purpose, we focus on anisotropic magnetic gels that contain chain-like aggregates of magnetic colloidal particles. Continuum elasticity theory is now used to describe the elastic behavior of the surrounding polymer matrix. Upon stretching along the chain direction, we predict a pronounced plateau-like ("superelastic") regime on the stress-strain curves. Remarkably, applying external magnetic fields, this plateau can be shifted along the stress-strain curves or even be switched off. We identify two underlying mechanisms: a detachment of the embedded chain-like aggregates and a flipping of the magnetic moments. The origin of both mechanisms is explained. It should be possible to observe these effects on real experimental samples and to exploit them, e.g., for the construction of soft actuators.

CPP 20.9 Tue 12:15 H51

Self-assembly properties of magnetic filaments in supracolloidal brushes — •Pedro A. Sánchez[1], Elena S. Pyanzina[2], Ekaterina V. Novak[2], Joan J. Cerdà[3], Tomas Sintes[3], and Sofia S. Kantorovich[1,2] — [1]University of Vienna, 1090 Vienna, Austria — [2]Ural Federal University, 620000, Ekaterinburg, Russia — [3]IFISC (UIB-CSIC), 07122 Palma de Mallorca, Spain

Magnetic filaments are chains of magnetic colloids that have been crosslinked with polymers to form permanent polymer-like structures. Recently, we proposed the use of these filaments to create supracolloidal magnetoresponsive coatings with a broad potential for technological applications [Sánchez *et al.*, Macromolecules 2015, 48, 7658–7669; Sánchez *et al.*, Faraday Discussions 2015, DOI:10.1039/c5fd00133a]. The proposed system is obtained by densely grafting the filaments to the coated surface, forming a polymer brush-like arrangement. Our computer simulations show that this system experiences strong equilibrium structural changes as a response to two main external parameters: background temperature and applied magnetic fields. The overall structure of the brush is determined by the self-assembly of the magnetic beads from neighbouring filaments under the influence of such external parameters. Importantly, the presence of the constrains introduced by the grafting surface and the crosslinkers makes this self-assembly significantly different from the one inherent to non crosslinked magnetic colloids in bulk.

CPP 20.10 Tue 12:30 H51

The effect of particle rearrangement in magneto-sensitive elastomers — •Dirk Romeis[1], Philipp Metsch[2], Markus Kästner[2], and Marina Saphiannikova[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V. — [2]Technische Universität Dresden

Magnetorheological elastomers are composites that consist of magnetically permeable particles incorporated into an elastic polymer matrix. When the magnetic field is applied to such material, changes in the shape and the mechanical moduli occur. The response of the material crucially depends on the actual distribution of the magnetizable particles and wether or not these particles can additionally rearrange with respect to the surrounding polymer network. We present a mean-field approach for initially statistically distributed magnetic dipoles and allow the formation of elongated microstructures in direction of the applied field. The results of the mean-field approach are compared with the predictions of a microscopic contiuum model of similar composites.

CPP 21: Hybrid and Perovskite Photovoltaics II (joint session CPP/DF/DS/HL, organized by CPP)

Time: Tuesday 10:45–13:00 Location: H37

CPP 21.1 Tue 10:45 H37

Charge Carrier Recombination Dynamics in Perovskite and Polymer Solar Cells probed by Time-Delayed Collection Field (TDCF) Experiments — •Andreas Paulke[1], Samuel D. Stranks[2], Juliane Kniepert[1], Jona Kupiers[1], Christian M. Wolff[1], Natalie Schön[1], Henry J. Snaith[2], Thomas J.K. Brenner[1], and Dieter Neher[1] — [1]Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht-Str.24-25, 14476 Potsdam — [2]Department of Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford OX1 3PU, United Kingdom

Time-Delayed Collection Field (TDCF) experiments are applied to organometal halide perovskite ($CH_3NH_3PbI_3$) based solar cells to investigate charge carrier recombination in a working solar cell at the nanosecond to microsecond timescale. Planar perovskite solar cells ($ITO/PEDOT:PSS/Perovskite/PCBM/C_{60}/BCP/Al$) display a second-order recombination process with a slow-down of the apparent recombination coefficient over several tens of nanoseconds. In contrast, recombination in the $ITO/TiO_2/mesoporous-TiO_2/Perovskite/Spiro-OMeTAD/Au$ device is governed by a slow first order process, but again with an apparent time-dependence of the recombination coefficient. We also conclude that organometal halide perovskite solar cells differ significantly from prototypical organic bulk heterojunction devices with regard to the mechanism and time-scale of free carrier recombination.

CPP 21.2 Tue 11:00 H37

Recombination of photogenerated charge carriers in planar methylammonium lead halide perovskite solar cells — •David Kiermasch[1], Stefan Väth[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

In the last years, solar cells based on organo-metal halide perovskites gained a lot of attention. The efficiency of solar cells with a perovskite absorber nowadays reaches more than 20%. With charge carrier mobilities up to tens of $cm^2V^{-1}s^{-1}$ and diffusion lengths exceeding 1 μm transport doesn't seem to be a limiting issue in this new kind of photovoltaic technology. However, recombination of the photgenerated charge carriers is an important factor defining e.g. the open circuit voltage of the solar cell. We prepared different methylammonium lead halide perovskite solar cells in planar configuration. Adressing the recombination dynamics, lifetime and concentration of photogenerated charge carriers are studied by transient photovoltage, charge extraction experiments as well as by the technique of open circuit voltage decay. We measured charge carrier lifetimes in the sub-μs-range for high illumination intensities ($\geq$ 1 sun), which is lower than in state of the art bulk heterojunction cells like P3HT:PCBM. Furthermore we discuss our results for different device morphologies and light-absorbing materials.

CPP 21.3 Tue 11:15 H37

Correlating charge carrier mobility, morphology and efficiency in hybrid halide perovskite photovoltaic devices — •Irene Grill[1,2], Michiel Petrus[1,2], Nadja Giesbrecht[1,2], Thomas Bein[1,2], Pablo Docampo[1,2], Matthias Handloser[1,2], and Achim Hartschuh[1,2] — [1]Department of Chemistry and CeNS, LMU Munich — [2]Nanosystems Initiative Munich (NIM)

Hybrid perovskites currently represent one of the most promising material systems for incorporation in future solar cell devices since their

efficiencies increased enormously in the last few years [1,2]. To date, fundamental physical properties including charge carrier dynamics and transport in these materials are not completely understood and are therefore at the focus of intense research. Here we extract the mobility of charge carriers in working thin film solar cells based on perovskite absorber layers and correlate it to the efficiency of the respective devices. To this end we performed Time-of-flight (ToF) studies on different perovskite thin films serving as photoactive layers. Further, in order to analyze the influence of contacts and other interfaces on charge transport and to identify possible optimization steps in the stacked architecture we carried out additional ToF measurements on each of the individual layers. Our results are discussed in terms of respective device efficiencies, morphologies and optical properties, allowing for a detailed investigation and identification of the limiting factors for the mobility and the efficiency in perovskite based thin film devices.
[1] M.A. Green and T. Bein, Nature Mater. 2015, 14, 559-561.
[2] N. Jeon et al., Nature 2015, 517, 476-480.

CPP 21.4 Tue 11:30 H37

Analysis of electronic trap states in methylammonium lead halide perovskite solar cells via thermally stimulated current — •Philipp Rieder[1], Andreas Baumann[1,2], Stefan Väth[1], Kristofer Tvingstedt[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, 97074 Würzburg

Organolead halide perovskite solar cells have emerged as one of the most promising technologies in thin-film photovoltaics due to their extraordinary increase in performance in only six years. Yet, the working principles of this material class still lack fundamental understanding. To address the possible influence of electronic traps on device performance, we probed solution processed methylammonium lead halide perovskite solar cells via thermally stimulated current (TSC) analysis.[1] Thereby, the sample is heated from 10 K to 300 K, while monitoring the current flow. This current is attributed to charge carriers being released from previously filled trap states in the semiconductor, allowing drawing conclusions about their distribution and energetic depth. Signals detected at low as well as at high temperatures can be attributed to shallow and deep traps, accordingly. Furthermore, a peak at around T=162 K can be assigned to the reported structural phase transition of the perovskite crystal from orthorhombic to tetragonal crystal lattice structure.

[1] A. Baumann et al., *J. Phys. Chem. Lett.* ***6****, 2350 (2015)*

15 min. break

CPP 21.5 Tue 12:00 H37

Tunable ferroelectric polarization and its interplay with spin-orbit coupling in tin iodide perovskite — Alessandro Stroppa[1], •Domenico Di Sante[2], Paolo Barone[1], Menno Bokdam[3], Georg Kresse[3], Cesare Franchini[3], Myung-Hwan Whangbo[4], and Silvia Picozzi[1] — [1]CNR-SPIN L'aquila, Italy — [2]CNR-SPIN L'aquila, Italy and Wuerzburg University — [3]Faculty of Physics, Center for Computational Materials Science, University of Vienna, Wien, Austria — [4]Department of Chemistry, North Carolina State University, USA

Ferroelectricity is a potentially crucial issue in halide perovskites, breakthrough materials in photovoltaic research. Using density functional theory simulations and symmetry analysis, we show that the lead-free perovskite iodide (FA)SnI$_3$, containing the planar formamidinium cation FA, (NH2CHNH2)$^+$, is ferroelectric. In fact, the perpendicular arrangment of FA planes, leading to a weak polarization, is energetically more stable than parallel arrangements of FA planes, being either antiferroelectric or strong ferroelectric. Moreover, we show that the weak and strong ferroelectric states with the polar axis along different crystallographic directions are energetically competing. Intriguingly, the relatively strong spin-orbit couling in noncentrosymmetric (FA)SnI$_3$ gives rise to a co-existence of Rashba and Dresselhaus effects and to a spin texture that can be induced, tuned and switched by an electric field controlling the ferroelectric state.

A. Stroppa, D. Di Sante et al., Nature Commun. 5, 5900 (2014)

CPP 21.6 Tue 12:15 H37

Mixed Pb:Sn methyl-ammonium halide perovskites: Thermodynamic stability and optoelectronic properties — •Lars Winterfeld, Ksenia Korshunova, Wichard J.D. Beenken, and Erich Runge — Institut für Physik, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Using density functional theory, we investigate systematically mixed $MA(Pb:Sn)X_3$ perovskites, where MA is $CH_3NH_3^+$, and X is Cl, Br or I. Our results cover optoelectronic properties, structural and thermodynamic stability. Ab initio calculations of the orthorhombic, tetragonal and cubic perovskite phases show that the substitution of lead by tin has a much weaker influence on both structure and cohesive energies than the substitution of the halogen. The thermodynamic stability of the $MA(Pb:Sn)X_3$ mixtures at finite, non-zero temperatures is studied within the Regular Solution Model. We predict that it will be possible to create iodide mixtures at any temperature. Mixing is unlikely for the low-temperature phase of bromide and chloride compounds, where instead local clusters are more likely to form. We further predict that in the high-temperature cubic phase, Pb and Sn compounds will mix for both $MA(Pb:Sn)Br_3$ and $MA(Pb:Sn)Cl_3$ due to the entropy contribution to the Helmholtz free energy. We calculated optoelectronic properties using both DFT and post-DFT methods (including self-consistent GW) with and without spin orbit coupling. Interestingly, the optoelectronic properties are not just a linear combination of the non-mixed parent structures and are not limited by the non-mixed values, which allows band gap engineering.

CPP 21.7 Tue 12:30 H37

A model Hamiltonian for perovskite solar cells — •Martin Schlipf, Marina R. Filip, Miguel A. Pérez-Osorio, and Feliciano Giustino — Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

Hybrid organic-inorganic halide perovskites emerge as one of most promising materials for new solar cells based on their high energy-conversion efficiency. The most commonly investigated materials include a large spin-orbit coupling, which may give rise to Rashba and Dresselhaus effects and makes them suitable for spintronic applications. In this contribution, we develop a simple model Hamiltonian that allows to study the impact of the spin-orbit coupling on the band structure. In particular, we focus on the physics near the bottom of the conduction band. Using group-theoretical considerations, we can reduce the number of parameters that the model exhibits. We apply this model to the prototype material MAPbI$_3$ (MA = CH$_3$NH$_3$) and show how different parameters of the model can be obtained from first-principles density functional theory (DFT) calculations. We discuss how the model can assist in designing improved perovskite solar cells.

CPP 21.8 Tue 12:45 H37

Stability and electronic properties of novel perovskites for photovoltaics from high-throughput ab initio calculations — •Sabine Körbel[1,2], Miguel A L Marques[2,3], and Silvana Botti[1,2] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Institut Lumière Matière, UMR5306 Université Lyon 1-CNRS, F-69622 Villeurbanne Cedex, France — [3]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

Using a high-throughput approach based on density functional theory, we perform an extensive search for stable ABX_3 perovskites, where X is a non-metallic anion and A and B are cations spanning the largest portion of the periodic table. Our search is motivated by the necessity to improve the thermodynamic stability of hybrid organo-metal halide perovskite absorbers. We calculate the ternary phase diagram for each composition and we discuss the thermodynamic stability of the perovskite phases. We find a large number of ABX_3 perovskites which are still absent from databases, and which are stable with respect to decomposition into known ternary, binary or elementary phases. For these structures, we then calculate electronic band gaps, hole effective masses, and the spontaneous ferroelectric polarization as relevant material properties for an application as photovoltaic absorbers. We find several novel perovskites which exhibit promising properties for photovoltaic applications. Based on our findings, we discuss possible strategies to improve the thermodynamic stability of perovskite absorbers.

CPP 22: Organic Electronics and Photovoltaics I (CPP/DS/HL/O, organized by CPP)

Time: Tuesday 14:00–15:30 Location: H37

CPP 22.1 Tue 14:00 H37

Elucidating the Morphology of Organic Bulk Heterojunction Solar Cells Using Nanoanalytical Transmission Electron Microscopy — •Stefanie Fladischer[1], Tayebeh Ameri[2], Christoph Brabec[2], and Erdmann Spiecker[1] — [1]FAU, CENEM, Erlangen, Deutschland — [2]FAU, i-MEET, Erlangen, Deutschland

Organic photovoltaics is one of the most promising technologies for low cost energy production with the advantages of semi-transparency, flexibility and solution processing. Significant improvement of the power conversion efficiency could be achieved in the last years using novel materials and adapted device engineering. To further improve the efficiency of solar cells the knowledge of the morphology is essential, as it decisively influences the device performance. The morphology of organic bulk heterojunction (BHJ) active layers depends not only on the involved materials but also on their molecular weight and their treatment like thermal annealing and solvent vapor annealing. Analytical Transmission Electron Microscopy (TEM) is a versatile tool to characterize the morphology of organic solar cells concerning on the one hand the interfaces of the various layers and on the other hand the material distribution in BHJ active layers. Combining high-resolution imaging with analytical techniques like electron energy-loss spectroscopy (EELS) and energy filtered TEM (EFTEM) as well as energy-dispersive X-ray spectroscopy (EDXS) the morphology can be determined and thus the device performance can be understood and further improved.

CPP 22.2 Tue 14:15 H37

Links between organic solar cell performance and morphological properties — •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, Munich School of Engineering, Herzig Group, 85748 Garching, Germany — [3]Elettra Sincrotrone Trieste S.C.p.A., Basovizza, 34149 Trieste, Italy

Many attempts have been made to establish solid links between morphology and performance of organic solar cells (OSCs) as well as the potential suitability of some materials for solar devices. Eventually, many of these attempts have yielded deeper insight into the physics governing excitonic solar cells. In this regard, one of the most innovative approaches consists in the in-operando observation of solar devices under working conditions in time-resolved grazing incidence X-ray scattering experiments. This configuration allows for simultaneous tracking of morphological and electronic properties as a function of time, making the appearing co-dependences among studied parameters more remarkable. The presented work focuses on the first in-operando observations that showed strong correlations between the crystalline state of P3HT:PCBM OSCs' active layers and the open-circuit voltage delivered by the devices. Up to now, this link was only addressed in a multi-step fashion with works featuring interdependences between properties like crystallinity, recombination, energy disorder, open-circuit voltage, or exciton/charge carrier transport.

CPP 22.3 Tue 14:30 H37

Strong influence of morphology on charge transport and recombination in solution processed small molecule based solar cells — •Alexey Gavrik[1], Andreas Baumann[2], Yuriy Luponosov[3], Sergey Ponomarenko[3,4], 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 — [3]Enikolopov Inst Synthet Polymer Mat, 117393 Moscow, Russia — [4]Lomonosov Moscow State University, 119991 Moscow, Russia

Solution processed small molecules (SSM) are promising materials for solar cell (SC) applications due to their well defined structure and high chemical reproducibility. Donor-acceptor-donor layout of SSM provides enhanced exciton splitting, as well as good possibility for effective charge transfer. The blend morphology in a bulk-heterojunction (BHJ) SC is assumed to play a crucial role in the cell performance. Therefore, we set to find optimal BHJ fabrication method keeping track of corresponding transport properties. In this work we studied $DTS(EtHex)_2$-$(2T\text{-}DCV\text{-}Me)_2$:$PC_{60}BM$ BHJ SC using the photogenerated charge carrier extraction technique OTRACE in order to analyze non-geminate recombination and determine charge carrier mobility in context of varying blend morphology. We show that different preparation conditions have a strong impact on the blend morphology and thus on the charge carrier transport (i.e. mobility and recombination rate). Furthermore, introduced modifications allowed to achieve a 4-fold enhancement of SC efficiency up to 4.3%.

CPP 22.4 Tue 14:45 H37

Direct visualization of charge-extraction in metal-mesh based OPV cells by light-biased LBIC — •Mathias Gruber[1,2], Arne Hendel[1], Vladislav Jovanov[1], Manfred J. Walter[2], and Veit Wagner[1] — [1]Department of Physics and Earth Sciences, Jacobs University Bremen, 28759 Bremen, Germany — [2]PolyIC GmbH & Co. KG, 90763 Fürth, Germany

Metal-mesh based electrode systems are a highly conductive, versatile and unexpensive alternative to ITO-electrodes for organic photovoltaic (OPV) cells. However, as a metal-mesh does not offer full surface conductivity it is usually combined with a less conductive PEDOT:PSS layer, which enables lateral charge-transport in the area in between the metal tracks. The sheet conductivity of this additional lateral conductive layer (LCL) needs to be carefully tuned with respect to the distance of the metal tracks to reduce short circuit current (J_{sc}) losses and additional series resistance due to resistive losses in the LCL material. Usually this is done via electrical simulation or via analysis of IV-measurements of a large number of devices with different LCL sheet conductivities. Here we present a direct way to measure the current collection losses due to PEDOT:PSS sheet resistance by integrating a white light-bias into a LBIC measurement (Light-bias LBIC). We show that we are not only able to directly measure and visualize charge extraction under real device operation conditions but are also able to determine the intrinsic PEDOT:PSS sheet resistance in the operating OPV device.

CPP 22.5 Tue 15:00 H37

Morphological Degradation of Polymer-Fullerene Bulk-Heterojunction Solar Cells — •Christoph J. Schaffer[1], Claudia M. Palumbiny[1], Martin A. Niedermeier[1], Christian Burger[1], Gonzalo Santoro[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

Organic solar cells offer a wide range of advantages based on their mechanical flexibility, their optical tunability and their ease of production in comparison to conventional photovoltaics. However, elongating their lifetime remains the main challenge after efficiencies exceeding the 10% marker have been recently reported [1]. We focus on the stability of the active bulk-heterojunction layer of polymer-fullerene solar cells. Using in-situ GISAXS and simultaneous current-voltage tracking we have previously shown that the active layer is morphologically unstable during operation of a P3HT:PCBM based solar cell, causing device degradation [2]. In our recent work we observe different degradation mechanisms occurring in other polymer-fullerene blends. This knowledge shows that tailored stabilization methods must be found for each specific material system.

[1] S.-H. Liao et al., Scientific Reports 2014, 4, 6813.
[2] C. J. Schaffer et al., Adv. Mater. 2013, 25, 6760.

CPP 22.6 Tue 15:15 H37

Illumination dependent parasitic resistances in organic bulk hetero junction solar cells. — •Arne Hendel and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

During outdoor operation, the solar cell is exposed to AM1.5G during noon only. For other daytimes and for indoor applications the performance of the solar cell at lower light intensities is important. In this study, bulk hetero junction solar cells were exposed to light irradiation from 10^{-5} to several suns intensity. We find a strong illumination dependence of the parasitic resistances. For the different light intensities I-V characteristics were performed. In addition the Jsc-Voc analysis was done to obtain series resistance free I-V measurement. It was found that the series and shunt resistance, which are critical for the solar cell performance, strongly depend on illumination intensity. The light intensity induced conductivity change of the solar cell shows different dependencies for forward and reverse operation. For low light intensities, the shunt resistance can be directly measured via the open circuit voltage assuming the Shockley model for the diode. From these measurements a strong light dependence is obtained. Based on the experimental data a model for the light dependent shunt resistance and series resistance is presented.

CPP 23: Charged Soft Matter

Time: Tuesday 14:00–15:30 Location: H40

CPP 23.1 Tue 14:00 H40

Ionic conductivity of plastic crystals — •Daniel Reuter, Korbinian Geirhos, Peter Lunkenheimer, and Alois Loidl — Experimental Physics V, University of Augsburg, Germany

Regarding the challenges of storing solar and wind energy or of electro mobility, the development of new solid-state electrolytes is often seen as a promising way to achieve further advances [1]. However, the development of a solid electrolyte with conductivity comparable to that of liquid electrolytes and mechanical properties of a solid is still in progress. There is a whole class of materials naturally combining properties of liquid and solid matter, namely the plastic crystals (PC). Below a certain transition temperature, the molecules of these materials form a well-defined crystalline lattice but still retain their orientational degrees of freedom. This feature of freely rotating molecules ordered in a crystalline structure is believed to enhance the mobility of dissolved ions in the material [2]. Remarkably, by adding a second component to one of the most prominent ionically conducting PCs, succinonitrile, an increase of the conductivity over several decades was found [3]. Therefore dielectric spectroscopy being sensitive to both molecular motion and ionic conductivity was applied to various molecular compositions of two-component PCs. We aim at answering the question if either the possible "revolving door" mechanism or defects in the lattice structure govern the high ionic charge mobility in these binary PC systems.

[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).

Invited Talk CPP 23.2 Tue 14:15 H40

Challenges and opportunities of nanostructured block copolymer membranes for lithium-ion batteries — •Ezzeldin Metwalli, Majid Rasool, Simon Brunner, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

The ionic conductivity in relation to the morphology of lithium-doped high-molecular-weight polystyrene-block-polyethylene oxide PS-b-PEO diblock copolymer films was investigated as solid state membranes for lithium ion microbatteries.[1] The tendency of the polyethylene (PEO) block to crystallize is highly suppressed with increasing both the salt doping level and the temperature. The PEO crystallites completely vanish at a salt doing ratio of Li/EO > 0.08, where the PEO segments are hindered from entering the crystalline unit of PEO chain. The increase of the lamella spacing D of the Li-ion/BC hybrid films with increasing Li salt doping level is attributed to the PEO chain conformation rather than the salt volume contribution or the previously reported increase of the effective interaction parameter. Upon salt upload, the PEO chains change from a compact/highly folded conformation to an amorphous/expanded-like conformation. The ionic conductivity is enhanced by the PEO amorphorization. We will further emphasize on the challenges related to the low conductivity of the Li-ion/BC membranes at room temperature which limit their practical implementation. Possible solutions are also suggested. [1] E. Metwalli et al., ChemPhysChem 16, 2882 (2015)

CPP 23.3 Tue 14:45 H40

Influence of DMSO-water solvent mixtures on counterion condensation behavior of lithium ions on sulfone based sulfonic acid based dimers. — •anand narayanan krishnamoorthy, christian holm, and jens smiatek — Institute for computational physics - University of Stuttgart

Molecular dynamics simulations were performed to study the solvation behavior of sulfone based sulfonic acid dimers in DMSO(Dimethyl sulfoxide) - water mixtures. Previous study show that the non ideality of the binary mixture solution is due to the cluster formation of DMSO and water molecules through hydrogen bonds between donor DMSO oxygen atom and hydrogen atom of water. This non-ideal behavior is also observed in ionic condensation behavior of lithium ions on dimer surface for specific mole-fractions of DMSO-water mixtures. It is seen that the activity of DMSO drives the counterion condensation behavior of lithium ion on the dimer surface. The non-ideal behavior, we observe can be related to solvent-solvent interactions and preferential solvation of the dimer and the counter ions. In addition the non-ideal nature of the pure DMSO-water mixture is also seen in the diffusive behavior of the solvents and reduced diffusivity is witnessed in presence of the solute(dimer) and qualitatively support the experimental results.

CPP 23.4 Tue 15:00 H40

Ion Pairing and Charging at Nanodroplet Surfaces in Oil/Water Emulsions — •Björn Braunschweig[1], Christian Sauerbeck[1], Andreas Krause[2], Frank R. Beierlein[2], Timothy Clark[2], and Wolfgang Peukert[1] — [1]Institute of Particle Technology — [2]Computer Chemistry Center, FAU Erlangen-Nürnberg

Molecular structures and interactions at oil/water interfaces are of great importance for emulsions and their properties such as stability or rheology. In our contribution, we demonstrate that not only the emulsifier coverage and structure, but also the solvation at the interface can significantly influence adsorption. Interfacial properties of emulsions were studied as function of sodium dodecyl sulfate (Na^+DS^-) and NaCl electrolyte concentrations. Experimental results from second-harmonic light scattering at the surface of nanodroplets with a mean radius of 83 nm were corroborated by extensive molecular dynamics (MD) simulations of hexadecane/water interfaces. We have experimentally determined the maximum surface excess of DS-anions (2.6 μmol/m^2) and the Gibbs free energy of adsorption (ΔG) in the presence of Na^+. Comparing 0 to 5 mM NaCl concentrations we show that ΔG changes from -34 to -41 kJ/mol. This change in ΔG is attributed to a formation of contact ion pairs (CIPs) between DS^- anions and Na^+ cations, which have a higher propensity to adsorb at the hexadecane/water interfaces. MD simulations clearly show that CIPs are formed and thus strongly corroborate conclusions from our experiments. In fact, MD simulations provide a more complete picture of Na^+, DS^- and water molecules at and near the interfacial region.

CPP 23.5 Tue 15:15 H40

Binding quantification by photochemically triggered microscale electrophoresis — •Friederike M. Möller, Michael Kiess, and Dieter Braun — Systems Biophysics, Nanosystems Initiative and Center for NanoScience, LMU Munich, Germany

Intricate feedback situations arise when chemical reactions are coupled to physical transport mechanisms. Self-organized patterns are well known for spatio-temporally controlled reaction-diffusion scenarios mostly in biology, but also in geology and chemistry. Here we use the light triggered dissociation of one reaction to create local electrical fields which enable the measurement of the association strength of another reaction.

In more detail, the photoactive compound o-nitrobenzaldehyde (o-NBA) dissociates upon UV irradiation and releases a proton. Differential diffusion of the charged photoproducts perturbs electroneutrality and generates a local electrical potential Φ on the low mV scale. Biomolecules move within the electrical field by electrophoresis. Due to backdiffusion on the microscale, concentration profiles settle within seconds proportional to $exp(-\mu/D\Delta\Phi)$. The diffusive character of transport makes the local, aqueous electrophoresis size selective.

We exploit the size selectivity for the quantification of aptamer-protein affinity in aqueous solution. Using the well characterized thrombin aptamer TBA15 as a proof of principle, we succeed in determining the K_D of binding in the nanomolar regime. Our results are in good agreement with literature and thermophoretic binding assays both with and without o-NBA.

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

Time: Tuesday 14:00–15:15 Location: H46

CPP 24.1 Tue 14:00 H46

Rheo-Chaos of Frictional Grains — •Matthias Grob, Annette Zippelius, and Claus Heussinger — Institut für Theoretische Physik, Georg-August Universität, Göttingen, Deutschland

A two-dimensional dense fluid of frictional grains is shown to exhibit time-chaotic, spatially heterogeneous flow in a range of stress values, σ, chosen in the unstable region of s-shaped flow curves. Stress controlled simulations reveal a phase diagram with reentrant stationary flow for small and large stress σ. In between no steady flow state can be reached, instead the system either jams or displays time dependent heterogeneous strain rates $\dot{\gamma}(\mathbf{r},t)$. The results of simulations are in agreement with the stability analysis of a simple hydrodynamic model, coupling stress and microstructure which we tentatively associate with the frictional contact network.

CPP 24.2 Tue 14:15 H46

From classical to quantum and back: A Hamiltonian scheme for adaptive multi-resolution classical/path integral simulations — •Karsten Kreis[1,2], Mark E. Tuckerman[3,4,5], Davide Donadio[1,6], Kurt Kremer[1], and Raffaello Potestio[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany — [3]Department of Chemistry, New York University (NYU), New York, NY 10003, USA — [4]Courant Institute of Mathematical Sciences, NYU, New York, NY 10012, USA — [5]NYU-East China Normal University Center for Computational Chemistry at NYU Shanghai, Shanghai 200062, China — [6]Department of Chemistry, University of California Davis, One Shields Ave., Davis, CA 95616, USA

Quantum delocalization of atomic nuclei affects the physical properties of many hydrogen-rich liquids and biological systems. To accurately model these effects, Feynman's path integral formulation of quantum statistical mechanics is typically employed, which implies a substantial increase in computational overhead. By restricting the quantum description to a small spatial region, this cost can be significantly reduced. Herein, we derive and validate a rigorous, Hamiltonian-based scheme that allows molecules to change from quantum to classical and vice versa on the fly as they diffuse through the system, both reducing overhead and making quantum grand-canonical simulations possible. Our adaptive resolution approach paves the way to efficient quantum simulations of biomolecules, membranes, and interfaces.

CPP 24.3 Tue 14:30 H46

All-Atom and Coarse-Grained Molecular Dynamics Simulation of Ionic Liquids — •Tamisra Pal and Michael Vogel — Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstrasse 6, 64289 Darmstadt

Room temperature Ionic Liquids (RTILs) have garnered much interest in the last few years as they possess tremendous potential for application in industry as reaction media. The high complexity of these liquids originating from their self-assembly or nano-scale aggregate formation motivates us to understand more on their dynamics. We have employed molecular dynamics simulation for RTILs to connect the length and time scales of simulation models with different levels of molecular resolution provided by the mapping scheme. Specifically, we have investigated a coarse grained (CG) model of 1-butyl-3-methylimidazolium hexafluorophosphate ([Bmim][PF_6]) and its all-atom (AA) description, at various temperatures. In this way, we unravel the different dynamical modes associated with dynamic heterogeneity and structural relaxation and we quantitatively compare the characteristic time scales from the two model systems to ascertain the effects of coarse graining on the dynamical behavior. The spatial and temporal aspects of molecular dynamics have been studied via calculating non-Gaussian parameters, particle displacement distributions, overlap functions and dynamic susceptibilities. Our simulation results provide a microscopic understanding to the presence of "fast" and "slow" moving particles contributing to dynamic heterogeneity and their relevance for the structural relaxation of ionic liquids.

CPP 24.4 Tue 14:45 H46

Equilibrium interfacial free energies and Turnbull coefficient for bcc crystallizing colloidal charged sphere suspensions — •Thomas Palberg[1], Patrick Wette[2,3], and Dieter M. Herlach[2] — [1]Institut f. Physik, Johannes Gutenberg Universität, 55099 Mainz, Germany — [2]Institut f. Materialphysik im Weltraum, DLR, 51147 Köln, Germany — [3]Space Administration, DLR, 53227 Bonn, Germany

The interfacial free energy (IFE) is a central quantity in crystallization from the meta-stable melt. In suspensions of charged colloidal spheres, nucleation and growth kinetics can be accurately measured from optical experiments. We here re-analyze the strictly linear increase of previously reported CNT-effective non-equilibrium IFEs estimated from such experimentsutilizing classical nucleation theory (CNT). For five aqueous suspensions of charged spheres and one binary mixture, we utilize a simple extrapolation scheme and interpret our findings in view of Turnbull's empirical rule. Our first estimates for the reduced equilibrium IFE, $\sigma_{0,bcc}$, between coexisting fluid and bcc-crystal phases are on the order of a few k_BT. Their values are not correlated to any of the electrostatic interaction parameters but rather show a systematic decrease with increasing size polydispersity and a lower value for the mixture as compared to the pure components. At the same time, σ_0 shows an approximately linear correlation to the entropy of freezing. The equilibrium interfacial free energy of strictly monodisperse charged spheres may therefore be still greater.

CPP 24.5 Tue 15:00 H46

Size matters: can we use a Hamiltonian adaptive resolution scheme to simulate an open system? — •Robinson Cortes-Huerto, Maziar Heidari, and Raffaello Potestio — Max Planck Institute for Polymer Research, Mainz, Germany

Finite size effects are ubiquitous in molecular dynamics simulations. Apart from the obvious implicit size effects due to periodic boundary conditions, explicit size effects are consequence of simulating a fixed and relatively small number of particles. In particular, measurements of density fluctuations within a sub-domain of a periodic simulation box are strongly dependent on the sub-domain size. These effects can be neglected by carrying out computer simulations for extremely large systems. An alternative solution is to use the Hamiltonian adaptive resolution scheme (H-AdResS), where the computational cost reduces substantially by embedding a relatively small high resolution portion of the system in a larger region at low resolution. Our main goal is to explore the viability to perform grand canonical simulations using this dual-resolution approach. In particular, we propose to use H-AdResS to calculate thermodynamic properties of prototypical molecular liquids in an effective open boundary simulation framework. To this end, we calculate Kirkwood-Buff integrals that connect radial distribution functions, available from molecular dynamics simulations, to thermodynamic properties such as the isothermal compressibility. We compare these results with measurements performed in the fully atomistic case and assess whether an adaptive resolution simulation reproduces the behaviour expected from an open simulation setup.

CPP 25: Focus: Functional Polymer Hybrids II

Time: Tuesday 14:00–16:00 Location: H51

Invited Talk CPP 25.1 Tue 14:00 H51

Plasmonic heating brings dynamic control of microgel shape and locomotion — •Ahmed Mourran, Hang Zhang, and Martin Moeller — DWI-Leibniz Institute for Interactive Materials, and Textile and Macromolecular chemistry, RWTH Aachen University Germany

Hydrogel actuation involves reversible swelling/shrinkage of the polymer network. However, the volume change of hydrogel is a slow diffusion-controlled process with a strong dependence on size. For this reason, hydrogels materials hardly allow instant control of their shape, making it difficult to develop fast and soft actuators. To overcome this limitation, we have combined non-equilibrium inhomogeneous swelling/shrinkage and anisometric microgel geometry to achieve large and fast bending deformations. An essential finding of this work is the generation of non-reciprocal actuation, i.e., each cycle consists of a forward and a distinct reverse movement, thereby creating the thrust needed to propel the hydrogel microswimmer in water. A body shape deformation is triggered by the photothermal heating of gold nanorods embedded in a temperature sensitive microgel. Absorption of high-intensity laser light by the plasmonic nanoparticles allows rapid heating and makes it possible to achieve fast dynamics. We will show that dynamic control of shape through plasmonics heating represents an exciting avenue in the development of photo-thermo-mechanical actuator or maneuverable soft microswimmers.

CPP 25.2 Tue 14:30 H51

Gold nanoparticles as local hot spots in thermoresponsive microgels — •Maren Lehmann, Weronika Nasiłowska, Tim Möller, Stefan Wellert, and Regine von Klitzing — Applied Physical Chemistry, TU Berlin, Berlin, Germany

Sensoric ultrathin coatings have a high impact in basic research and for technical applications. A promising combination is of metal particles embedded in a polymer matrix. The metal particles can interact with external fields (e.g. light, magnetic field) and the polymer matrix can be sensitive to outer stimuli like temperature, pH or ionic strength. Here, we present a hybrid system of thermosensitive poly(N-isopropylacrylamide) (PNIPAM, LCST: 32°C) microgels and Au nanoparticles (Au NP). The incorporation of Au NP into the PNIPAM microgel influences the optical properties of the microgels via plasmon coupling during their volume phase transition [1] [2]. In order to study the effect of hot spots, we coupled a second laser for plasmon excitation into our dynamic light scattering (DLS) set-up. The loading density of the Au NP within the microgels was optimized for our purpose. The plasmon excitation of Au NP results in local heating providing enough heat to induce a reduction in the microgel size. Depending on the uptake of Au NP the induced size change also varies and the apparent internal temperature within the gel can be determined.

1. Lange, H. et al. Langmuir, 2012, 28, 8862
2. Gawlitza, K. et al. Phys. Chem. Chem.Phys., 2013, 15, 15623

CPP 25.3 Tue 14:45 H51

Thermal Transport in Colloidal Crystals and Assemblies — Fabian A. Nutz^{1}, Pia Ruckdeschel^{1}, Alexandra Philipp^{1}, Tobias Kemnitzer^{2}, Jürgen Senker^{2}, and •Markus Retsch^{1} — ^{1}Physical Chemistry - Polymer Systems, University of Bayreuth, 95447 Bayreuth, Germany — ^{2}Inorganic Chemistry III, University of Bayreuth, 95447 Bayreuth, Germany

We will present our latest results on thermal transport phenomena in colloidal materials, which are structured on length scales that bridge 10 nm up to 1 um. We will particularly introduce two examples of so-called colloidal crystals, which comprise either monodisperse polystyrene particles, composite core/shell spheres, or hollow silica capsules. While being entirely amorphous on a local scale, colloidal crystals feature opalescent colors due to their highly crystalline order on a couple of 100 nm. Such systems are well suited to investigate fundamental structural changes on an individual particle level and their influence on the effective thermal conductivity of the colloidal superstructure. We demonstrate the influence of microporosity and interfacial adhesion to the thermal transport in silica hollow spheres.[1] Polymer colloidal crystals are insensitive to their surrounding atmosphere but exhibit a strong hysteresis upon film formation.[2] [1] P. Ruckdeschel, et al., Nanoscale, 2015, 7, 10059 [2] F. A. Nutz, et al., J. Coll. Interf. Sci., 2015, 457, 96

15 min. break

CPP 25.4 Tue 15:15 H51

Network topology in magnetic gels studied by simulating the cross-linking process — •Rudolf Weeber and Christian Holm — Institut Fuer Computerphysik, Universitaet Stuttgart, Allmandring 3, 70569 Stuttgart

Ferrogels are hydrogels into which magnetic nanoparticles are immersed. Thereby,they combine elastic properties with the ability to react to external magnetic fields, which makes them candidates for applications such as drug delivery and actuation. One aspect of ferrogels, which is expected to have a large influence on their properties, is the topology of the polymer network forming the gel. This is, however, difficult to access experimentally. We therefore study the question using computer simulations. In the contribution, we present simulations of the cross-linking process of a magnetic gel, and we examine, how the resulting gel changes, depending on the conditions during cross-linking.

CPP 25.5 Tue 15:30 H51

structure and dynamics of nanocomposite hydrogels based on HEUR polymers and coated magnetite nanoparticles. — •Antonella Campanella^{1}, Olaf Holderer^{1}, Konstantinos Raftopoulos^{2}, Peter Müller-Buschbaum^{2}, and Henrich Frielinghaus^{1} — ^{1}JCNS@FRMII, Lichtenbergstrasse 1, 85747 Garching, Germany — ^{2}Technische Universität München, Physik-Department, LS Funktionelle Materialien, James-Franck-Strasse 1, 85748 Garching, Germany

Magnetic nanoparticles as component in the nanocomposite hydrogel formulation lead to a wide variety of applications, e.g. cancer treatment, separation devices, electromagnetic waves absorbers. The structure and the dynamics of nanocomposite hydrogels based on HEUR (hydrophobically modified ethoxylated urethanes) polymers and coated magnetite magnetite nanoparticles are investigated with small angle neutron scattering (SANS) and with dielectric relaxation spectroscopy (DRS) in combination with neutron spin echo (NSE), respectively. The embedding of the magnetite nanoparticles in the HEUR polymer network leads to i) an increase of the domain spacing of the polymer network, i.e. the distance between the hydrophobic domains composed of the alkyl ends of the HEUR polymer and ii) a partial suppression of the segmental motion of the middle polar block of the HEUR polymer.

CPP 25.6 Tue 15:45 H51

Multiresponsive PNIPAM Microgels Doped with Magnetic Nanoparticles — •Marcus U. Witt^{1}, Sebastian Backes^{1}, Eric Roeben^{2}, Birgit Fischer^{3}, Annette M. Schmidt^{2}, and Regine v. Klitzing^{1} — ^{1}Technische Universität Berlin, Institut für Chemie, Stranski Laboratorien, Straße des 17. Juni 124, 10623 Berlin — ^{2}Universität zu Köln, Institut für Physikalische Chemie, Luxemburger Straße 116, 50939 Köln Gebäude 322 — ^{3}Universität Hamburg, Institut für Physikalische Chemie, Grindelallee 117, 20146 Hamburg

N-isopropylacrylamide (NIPAM) based microgels exhibit a volume phase transition temperature (VPTT) at approximately 32°C. This VPTT leads to a reversible swelling and shrinking in water due to changes in temperature. There are several co-monomers which can be added to achieve additional responsive parameters such as pH or the ionic strength. To make the gels responsive to an external magnetic field we incubated magnetic nanoparticles (MNP) in the gel structure (ferrogel). In the present study different synthesis strategies are applied for the fabrication of homogenous and heterogeneous microgels. The effect of MNP loading due to the internal structure is studied. The investigation governs the thermoresponsive behavior of the ferrogel, the distribution of the MNP inside the gel matrix and the response to a static magnetic field in bulk and at a solid surface.

CPP 26: Poster: Charged Soft Matter, Polyelectrolytes, Ionic Liquids

Time: Tuesday 18:15–21:00 Location: Poster B2

CPP 26.1 Tue 18:15 Poster B2

Static dielectric properties of dense ionic fluids — •Grigorii Zarubin[1,2] and Markus Bier[1,2] — [1]Max Planck Institute IS — [2]University of Stuttgart

In order to interpret surface force apparatus measurements recent experimental work [1] suggests that room temperature ionic liquids (RTILs) can be viewed as dilute electrolyte solutions with a few mobile ions in an effective solvent made of temporary paired ions. In this work we attempt to answer whether this model is viable looking at RTILs from the point of view of their dielectric properties.

Using calculated electrical susceptibility $\chi(k) = \varepsilon(k) - 1$ we showed [2] that RTILs are expected to behave plasma-like on sufficiently long distances however exhibiting dipolar fluid-like dielectric properties for small separations. Thus, the recently debated interpretation of RTILs as dilute electrolyte solutions [1] might not be simply a yes-no-question but it might depend on the considered lengthscale.

[1] M. Gebbie et al., Proc. Natl. Acad. Sci. U. S. A. **110**, 9674 (2013)
[2] G. Zarubin and M. Bier, J. Chem. Phys. **142**, 184502 (2015)

CPP 26.2 Tue 18:15 Poster B2

Self-assembled hybrid materials as a membrane for lithium-ion batteries — •Simon Schaper, Ezzeldin Metwalli, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Lithium-ion batteries are the state of the art solution powering portable electronic devices, electrically driven vehicles and storing homemade solar energy. The morphology and conductivity of a high molecular weight polystyrene-block-polyethylene oxide (PS-b-PEO) block copolymer containing lithium salt and titania nanoparticles were investigated at different temperatures. The crystallization of the PEO block was highly suppressed at a certain Li-salt doping level as well as upon increasing titania concentration. SAXS measurements indicate a morphological transition from lamella to cylinders and spheres with subsequent solid-state hybrid membrane amorphization. The conductivity behavior of the hybrid membrane is correlated to the membrane structure. A proper amount of titania nanoparticles suppresses also the dendrite growth of the battery electrodes and therefor enhances the cycling stability of the cell.

CPP 26.3 Tue 18:15 Poster B2

Multiresponsive hydrogels from telechelic polyelectrolytes — •Chia-Hsin Ko[1], Margarita A. Dyakonova[1], Sandra Gkermpoura[2], M. M. Soledad Lencina[2], Constantinos Tsitsilianis[2], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]University of Patras, Department of Chemical Engineering, Patras, Greece

Multiresponsive polymeric hydrogels offer a rich switching behavior. We investigate the structural properties of self-assembled pH- and thermo-responsive hydrogels from ABA triblock terpolymers, bearing a pH-responsive central block and thermo-responsive hydrophobic end blocks P(nBuMA-co-TEGMA)-b-PDMAEMA-b-(nBuMA-co-TEGMA) (nBuMA, TEGMA and DMAEMA are n-butyl methacrylate, tri-(ethylene glycol)methyl ether methacrylate and 2-(dimethylamino)ethyl methacrylate). Varying temperature, it is possible to alter the water-solubility of TEGMA and, thus, to influence the exchange dynamics of the stickers. The rheological properties of hydrogels have been found to depend strongly on pH and temperature. A transition from a dynamic hydrogel network to a kinetically frozen network upon increase in temperature was indeed found. pH variation significantly affects the dynamic behavior of formed hydrogels because it alters the degree of stretching of the middle PDMAEMA block. In order to investigate the internal architecture of the hydrogels, we perform small-angle X-ray scattering (SAXS) in dependence on pH and temperature.

CPP 26.4 Tue 18:15 Poster B2

Combing polyelectrolyte brushes with polyelectrolyte multilayer: A neutron reflectivity study in humid conditions — •Oliver Löhmann[1], Samantha Micculla[1], Olaf Soldwedel[2], and Regine von Klitzing[1] — [1]Technische Universität Berlin — [2]Max Planck Institut für Festkörperforschung Stuttgart

Polyelectrolyte brushes and polyelectrolyte multilayer (PEM) are two powerful approaches to modify surfaces. Both have their advantages due to their different geometrical orientation and their different binding to the surface. A combination of both can favor special properties. The covalent binding of the polymer brush to surface can lead to a long stability. The diversity of PEM results in an enormous variety of stimuli responsive coatings. Here, a combination of the well-known PMETAC brush and PSS/PDADMAC PEM is investigated. Neutron reflectivity is used to get information about swelling behavior and the interdigitation while changing the humidity. Therefore, a contrast between the interface is generated by deuterating the PEM.

Here, we show the impact of humidity on the system. The combined system do not swell like the separate ones. The total system can be separated in two regimes: brush and PEM regime. The brush regime absorbs more water than the PEM regime but not as much as an uncoated brush. Additionally, the amount of PEM, which is diffused into the brush, can be calculated.

CPP 26.5 Tue 18:15 Poster B2

Cluster formation in protein solutions with trivalent salts investigated by light scattering — •Michal Braun, Olga Matsarskaia, Daniel Soraruf, Fajun Zhang, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen

The formation of clusters or small aggregates in protein solutions with (partly) attractive interactions is considered an unsolved issue. Salt ions offer a way to manipulate the interaction with a high degree of control. In a variety of protein-(multivalent) salt systems reentrant condensation has been found. For a fixed protein concentration the solution is clear below a salt concentration c^*, then becomes turbid (so-called regime II) and redissolves again above c^{**}. Aggregates, possible precursors of crystallization, and their diffusion behavior were recently studied in a system that phase separates macroscopically between c^* and c^{**}. The diffusion behavior there points to c^* being a spinodal line which can be deduced from the fact the collective diffusion coefficient D becomes zero at c^* [1]. Here a light scattering study of a system is presented where there is no macroscopic phase separation at room temperature, only slight turbidity in regime II. D also decreases steeply towards a c^* where it attains its minimum value but remains finite. In regime II D stays constant and then starts to increase again slowly.

[1] Soraruf et al., *Soft Matter*, **10**, 894, 2014

CPP 26.6 Tue 18:15 Poster B2

A coarse-grained model for polyionic liquids — •Alexander Weyman[1], Jens Smiatek[1], Markus Bier[2], and Christian Holm[1] — [1]Institut für Computerphysik, Universität Stuttgart, Germany — [2]Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany

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. [1]

We show first results from molecular dynamics 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.

We intend to calculate the dynamic and static structure factor for single chains and for dense polymer solution to gain insights into structural properties. This will allow us to compare our results to experimental data.

[1] Yuan et al., Poly(ionic liquid)s: An update, Progr. Polym. Sci. 38 (2013) 1009-1036

CPP 26.7 Tue 18:15 Poster B2

Surface Segregation of Alkanes in Ionic Liquids — •Julian Mars[1,2], Henning Weiss[2], Hailong Li[2], Bridget Murphy[3], and Markus Mezger[1,2] — [1]Johannes Gutenberg-Universität Mainz, Germany — [2]Max-Planck-Institut für Polymerforschung, Mainz, Germany — [3]Christian-Albrechts-Universität zu Kiel, Germany

Ionic Liquids (ILs) are promising candidates in a variety of applications such as heterogeneous catalysis. In the SILP (Supported Ionic Liquid

Phase) catalysis the chemical reaction takes place in a thin IL film, wetting a solid support material with high surface area. Recently, it has been proposed that the observed performance degradation is related to aggregation of side products at the IL/gas interface, forming diffusion barriers for educts and products. As a model system, we studied the near surface structure of an alkane containing IL by x-ray reflectivity. Analysis of the experimental data revealed surface segregation of the alkanes, affecting the interfacial ion profile.

CPP 26.8 Tue 18:15 Poster B2

Analysis of the radiation-induced degradation of the ionic liquid [EMIm]Tf2N by use of quantum-chemical fragment calculations — Marcus Reinmöller[1], Angela Ulbrich[2], Stefan Krischok[2], and •Wichard J. D. Beenken[2] — [1]TU Bergakademie Freiberg, Institut für Energieverfahrenstechnik und Chemieingenieurwesen, Fuchsmühlenweg 9, 09599 Freiberg — [2]Technische Universität Ilmenau, Institut für Physik, Weimarer Straße 32, 98693 Ilmenau

The radiation-induced degradation of the room-temperature ionic liquid [EMIm]Tf2N by X-rays has resulted in time-dependent shifts of the XPS core level Peaks [1]. These shifts can be regarded as fingerprints of the formed fragments of the ions as well as hints towards the present degradation mechanisms. Reconstruction of XPS spectra by means of a Gelius type approach based on DFT calculations with an appropriate energy rescaling [2,3] allows us to identify several charge- and spin-compensated fragments from the initial ion pair. Thus an analysis of the degradation mechanisms on the atomic scale is made, which is in agreement to the results of the experimental XPS study [2]. For example, bond breakage inside the anion has preferentially appeared next to the central nitrogen whereas the cation degenerates mostly by breaking off the alkyl sidechains.

[1] Keppler, A. *et al. Phys. Chem. Chem. Phys.* **13** (2011) 1174

[2] Reinmöller, M. *et al. Phys. Chem. Chem. Phys.* **13** (2011) 19526

[3] Ulbrich, A. *et al J. Mol. Liq.* **192** (2014) 77

CPP 26.9 Tue 18:15 Poster B2

Branched Poly(ethylenimine) as Barrier Layer for Polyelectrolyte Diffusion in Multilayer Films — Peter Nestler[1], Malte Passvogel[1], •Heiko Ahrens[1], Olaf Soltwedel[2], Ralf Köhler[3], and Christiane A. Helm[1] — [1]University Greifswald, 17487 Greifswald, Germany — [2]MPI for Solid State Research, 70569 Stuttgart, Germany — [3]HZB, 14109 Berlin, Germany

Polyelectrolyte multilayer films are made by sequential adsorption of polyanions and polycations from 0.1 mol/L NaCl. Their internal structure is investigated with neutron reflectivity. The films are made from poly(ethylenimine) (PEI), poly(diallyldimethylammonium) (PDADMA) and poly(styrenesulfonate) (PSS respective deuterated PSSd). Each film consists of a protonated and a deuterated block, built from m protonated and n deuterated polycation/polyanion layer pairs, respectively. The films are annealed in salt solution (1 mol/L NaCl). During annealing of PDADMA/PSS films the internal interface between the two blocks broadens due to interdiffusion, thus the PSS diffusion coefficient is measured. Eventually the annealing leads to a uniform distribution of protonated and deuterated PSS throughout the PDADMA/PSS film. Yet, if one polycation layer in the film centre is branched PEI, then this PEI layer serves as a diffusion barrier, which is impenetrable for up to a third of PSS. The equilibration time of the remaining mobile PSS fraction increases which is attributed to the low permeation rate through the barrier layer. Possibly, some PSS molecules have a conformation that hinders them to cross the barrier layer, or the barrier layer gets clogged with time.

CPP 27: Poster: Soft Matter Dynamics / Glasses

Time: Tuesday 18:15–21:00 Location: Poster B2

CPP 27.1 Tue 18:15 Poster B2

Fragile-to-strong transition in liquid silica — •Julian Geske, Barbara Drossel, and Michael Vogel — Institut für Festkörperphysik, Technische Universität Darmstadt

We investigate anomalies in liquid silica with molecular dynamics simulations and present evidence for a fragile-to-strong transition at around 3000K. To this purpose, we studied the structure and dynamical properties of silica over a wide temperature range, finding three indicators of the fragile-to-strong transition. First, there is a density minimum at around 3000K and a density maximum at 3400K. Second, the local structure characterized by the tetrahedral order parameter changes dramatically around 3000K and changes from a higher-ordered, lower-density phase to a less ordered, higher-density phase. Third, the correlation time τ changes from an Arrhenius behaviour below 3000K to a Vogel-Fulcher behaviour at higher temperatures.

CPP 27.2 Tue 18:15 Poster B2

Molecular Mobility and Gas Transport Properties of PIM-1 and Nano composites based on PIM-1 and PhenethylPOSS — Nora Konnertz, Yi Ding, Martin Böhning, and •Andreas Schönhals — Bundesanstalt für Materialforschung und -prüfung (BAM), Unter den Eichen 87, 12205 Berlin

Polymers with intrinsic microporosity are of highly interest in the field of gas separation membranes. Especially the first synthesized PIM-1 shows extraordinary permeabilities and selectivities. Unfortunately, PIM-1 tends to physical aging and loses its good properties. Physical aging is related to the molecular mobility of PIM-1 which was here investigated by broadband dielectric spectroscopy (BDS). Besides the studies on pure PIM-1 a polyhedral oligomeric silsesquioxane with phenethyl substituents (PhenethylPOSS) was used as nanofiller (0 - 40 wt-%) in the PIM-1 matrix to improve the gas transport properties and prevent physical aging. The molecular mobility of the solution casted nano composite films was analyzed by BDS as well. Furthermore, gas transport properties were determined with the time lag method (0 - 20 bar) in a temperature range of 35°C to 65°C with N2, O2, CH4 and CO2.

CPP 27.3 Tue 18:15 Poster B2

Dynamical coexistence in polydisperse hard spheres — •Matteo Campo and Thomas Speck — Institut für Physik, JGU Mainz, Germany

We investigate the slow dynamics of a model glass former, the polydisperse hard-sphere liquid, using a combination of molecular dynamics and importance sampling in the trajectory ensemble. According to dynamical facilitation theory, the glass transition takes place as a consequence of dynamical heterogeneity which develops as the liquid is quenched. We characterize dynamical heterogeneity by a parameter, the mobility, which quantifies how far particles move in the supercooled liquid. By studying trajectories longer than the structural relaxation time, we observe exponential tails in the probability distribution of mobility, which indicate phase coexistence of normal and exceptionally slow trajectories.

CPP 27.4 Tue 18:15 Poster B2

Time needed to form stable glasses is comparable to β-relaxation time — •Yeong Zen Chua, Mathias Ahrenberg, and Christoph Schick — Institute of Physics, University of Rostock, Rostock 18051 Germany

Glasses produced by physical vapor deposition (PVD) exhibit different properties, depending on the deposition conditions. Consistent with previous works, glasses of ethylcyclohexane (ECH) vapor-deposited at temperature of about 0.85 of glass transition temperature, T_g observed to be the most stable glasses with low enthalpy, low heat capacity, high kinetic stability and high density. Isothermal transformation of the as-deposited glasses into the supercooled state is investigated for the deposition rate dependency, covering four orders of magnitude, at different substrate temperatures. The kinetic stability of the glasses (transformation time at 103 K) shows strong deposition rate dependency for lower substrate temperatures. The data provide an estimate for the substrate temperature dependent free surface residence time needed for the molecules in the assumed mobile surface layer to promote stable glass formation. Stable glasses are formed if this time is of the order of the β-relaxation time, many orders of magnitude faster than the α-relaxation at the substrate temperature. Stable glasses are observed even for substrate temperatures below the Vogel and the Kauzmann temperatures, indicating a full decoupling of the process of stable glass formation from the α-relaxation.

CPP 27.5 Tue 18:15 Poster B2

Diffusion of PMMA: microgels and linear polymer — •Bastian Pur[1], Werner Köhler[1], Klaus Huber[2] und Martin Schneider[2] — [1]Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Physikalische Chemie, Universität Paderborn, 33098 Paderborn, Germany

In present theories for polymer thermophoresis in dilute solutions there are two theoretical models under discussion: draining coil and nondraining coil, corresponding to the Rouse and the Zimm picture, respectively. In order to discriminate between these models we have started a comparative investigation of a linear chain polymer and cross-linked microgels. The linear polymer sample used is poly(methylmethacrylate) (PMMA) and the micro-gel samples are PMMA cross-linked with different amounts of ethylen-di-methacrylate (EGMA). In either case toluene is used as solvent. By means of transient holographic grating technique we obtained the thermal diffusion coefficient D_T , the Fickian diffusion coefficient D and the Soret coefficient S_T as functions of the polymer concentration c. We have found out that for $c \to 0$ the hermophoretic mobility of the linear polymer and the microgel with 3.5% EGMA are identical within experimental accuracy. In addition we performed dynamic light scattering experiments to characterize the different microgel samples. Thereby we obtained that the diffusion coefficient is independent of the amount of cross-linker and so are (by using Stokes-Einstein equation) the hydrodynamic radii of the microgels.

CPP 27.6 Tue 18:15 Poster B2

Diffusion of PMMA: microgels and linear polymer — •Bastian Pur[1], Werner Köhler[1], Klaus Huber[2] und Martin Schneider[2] — [1]Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Physikalische Chemie, Universität Paderborn, 33098 Paderborn, Germany

In present theories for polymer thermophoresis in dilute solutions there are two theoretical models under discussion: draining coil and nondraining coil, corresponding to the Rouse and the Zimm picture, respectively. In order to discriminate between these models we have started a comparative investigation of a linear chain polymer and cross-linked microgels. The linear polymer sample used is poly(methylmethacrylate) (PMMA) and the microgel samples are PMMA cross-linked with different amounts of ethylen-di-methacrylate (EGMA). In either case toluene is used as solvent. By means of transient holographic grating technique we obtained the thermal diffusion coefficient D_T, the Fickian diffusion coefficient D and the Soret coefficient S_T as functions of the polymer concentration c. We have found out that for $c \to 0$ the thermophoretic mobility of the linear polymer and the microgel with 3.5% EGMA are identical within experimental accuracy. In addition we performed dynamic light scattering experiments to characterize the different microgel samples. Thereby we obtained that the diffusion coefficient is independent of the amount of cross-linker and so are (by using Stokes-Einstein equation) the hydrodynamic radii of the microgels.

CPP 27.7 Tue 18:15 Poster B2

Extracting material net properties of monomolecular coverages from broadband dielectric spectroscopy measurements with nano-structured electrode arrangements — •Martin Tress[1,2], Nils Neibauer[2], Rene Winkler[3], Petra Uhlmann[3], Emmanuel Mapesa[2], Manfred Reiche[4], and Friedrich Kremer[2] — [1]Max Planck Institute for Polymer Research, Mainz — [2]University of Leipzig — [3]Leibniz-Institut für Polymerforschung Dresden e.V. — [4]Max Planck Institute of Microstructure Physics, Halle (Saale)

Recently, Broadband Dielectric Spectroscopy (BDS) has been combined with a nano-structured electrode arrangement to investigate glassy dynamics in monomolecular layers and isolated polymer chains [1]. Thereby, insulating nano-structures serve as spacers between the silicon electrodes enabling an electrode separation of only 40 nm. Since this is still larger than the height of the actual sample material, a major fraction of the capacitor volume is empty. Consequently, the measured signal is an average of several contributions, including the dielectric properties of the sample itself, the spacer material and the gap between the electrodes. Due to the particular geometry, the composition of these contributions is not straight-forward. To unravel the individual dielectric functions of all components an equivalent circuit model is employed. Using BDS spectra of poly(2-vinylpyridine) (P2VP) brushes and condensed isolated P2VP chains as examples it is demonstrated how to unravel molecular relaxations, polarization effects and charge transport as well as the extraction of their net properties.

[1] M. Tress et al. Science 341 (2013) 1371

CPP 27.8 Tue 18:15 Poster B2

Molecular Dynamic Simulation and forcefield creation of Poly(3-hexylthiophene) for aggregation investigations — •Marie Kathrin Tritschel and Stephan Gekle — Universität Bayreuth

Poly(3-hexylthiophene) is a widely investigated polymer for light harvesting devices as it possesses comparably good performances due to its high charge carrier mobility.

Using molecular dynamics simulation we show that there is a temperature dependent aggregation between different polymer chains in agreement with corresponding spectroscopic experiments.

Additionally investigations of the ordering and the packing behaviour of the chains are performed in atomistic and coarse grained representations of the system.

CPP 28: Poster: Computational Physics of Soft Matter

Time: Tuesday 18:15–21:00 Location: Poster B2

CPP 28.1 Tue 18:15 Poster B2

Dimensionality aware method for the domain decomposition of homogeneous and inhomogeneous molecular dynamics simulations — •Horacio V. Guzman, Torsten Stuehn, and Kurt Kremer — Ackermannweg 10, 55128 Mainz

Molecular simulations are a scientific tool that has enabled theoretical and computational methods to tackle soft matter research. This is reflected in the permanent development and enhancement of new methodologies within scientific codes[1,2,3]. One of the challenges in molecular dynamics simulations is to improve efficiency in the parallelization of domain decomposition schemes. Here, we present a new iterative method to optimize the decomposition of the simulation box which combines the dimensionality of the system and the level of parallelization to be used. In addition the proposed method also includes a shifting domain walls feature for an adpatative load balancing of inhomogeneous systems[4]. We have implemented the method in ESPResSo++[1] which allowed us to benchmark both homogeneous[5] and inhomogeneous systems. By comparing the existing domain decomposition scheme[1] with the new dimensionality aware method, we prove that the latter enables a computationally more efficient domain decomposition for both homogeneous and inhomogeneous systems, and hence a speedup increase, as well as, a higher upper bound scaling. [1] J. D. Halverson et al., Compt. Phys. Comm. 184 (2013) [2] W. M. Brown et al., Comput. Phys. Comm. 195 (2015) [3] B. Hess et al., J. Chem. Theory Comput. 4 (2008) [4] M. Praprotnik et al., Phys. Rev. E 73 (2006) [5] L. Moreira et al., Macromol. Theory Simul. 24(2015)

CPP 28.2 Tue 18:15 Poster B2

SAMC simulation of single peptides in the PRIME20 model — •Arne Böker and Wolfgang Paul — Martin-Luther-Universität Halle-Wittenberg

A number of current problems in medical science can be attributed to misfolding of proteins when these reach non-native free energy minima stabilized by aggregation. Describing these aggregation phenomena for relevant protein sizes requires the use of coarse-grained models. However, strongly coarse-grained computational models tend to simplify the free energy surface in such a way that these local minima are suppressed. To circumvent this problem, the level of coarse graining needs to be chosen appropriately.

PRIME20[1] is an intermediate-resolution model for proteins. It provides reasonable detail by mapping each amino acid to four beads, but keeps parameter space relatively simple with the set of interactions reduced to 19 parameters. We perform thermodynamic simulations of single PRIME20 chains using the "SAMC"[2] variation of Wang-Landau Monte Carlo samplng which provides insight in different statistical ensembles at the expense of dynamic information.

[1] M. Cheon, , I. Chang, C. K. Hall, Proteins **78**(2010):2950

[2] B. Werlich, T. Shakirov, M. P. Taylor, W. Paul, Comp. Phys. Comm. **186**(2015):65

CPP 28.3 Tue 18:15 Poster B2

Stiffness of Homopolymer Chains — •Benno Werlich[1], Timur Shakirov[1], Mark P. Taylor[2], and Wolfgang Paul[1] — [1]Institut für Physik, Martin-Luther Univerität Halle-Wittenberg, Halle (Saale) — [2]Department of Physics, Hiram College, Ohio, USA

For studying structure formation of homopolymer chains we use an off-lattice hard-sphere coarse grained model with square-well interactions. The indication of first and second order like pseudophase-transitions has been done with the help of microcanonical and canonical analysis. Therefore, a stiffness dependent state-diagram is shown for 40-mers. An example of various chain lengths for fixed stiffness shows an evolution of pseudophase-transitions. Beside nonspecific square-well interactions we introduced additional specific square-well interactions and study its effects. The simulations have been performed with the help of the Stochastic Approximation Monte Carlo Method (SAMC). SAMC is a type of Wang-Landau Monte Carlo.

CPP 28.4 Tue 18:15 Poster B2

Differences in the structural flexibility of the sulfur and oxygen mustards molecules from Car-Parrinello molecular dynamics simulations — •Joanna Lach[1], Pawel Rodziewicz[2], Mariana Kozlowska[2], and Maciej Baradyn[2] — [1]Faculty of Physics, Vilnius University, Lithuania — [2]Institute of Chemistry, University of Bialystok, Poland

Sulfur mustard (SM) is an organic blister chemical warfare agent (CWA). It was thought that huge amounts of water can neutralize CWAs, thus after II World War large amounts of CWA were dumped into the Baltic Sea. Due to the high toxicity, SM, was often replaced with its structural analogue, namely, oxygen mustard (OM).

The conformational analysis of the SM and OM molecules was performed utilizing ab initio calculations. The dynamics of the system and all structural rearrangements between the local and global minima were studied at finite temperature by Car-Parrinello molecular dynamics (CP-MD) simulations. Post-processing population analysis of the relative low energy conformations was carried out. The existence of the most probable rearrangements was investigated. Crucial differences between structures of global and local minima for both SM and OM molecules were reported.

CPP 28.5 Tue 18:15 Poster B2

FT-IR matrix isolation and theoretical study of tetrahydrofuran pseudorotation — •Joanna Lach[1], Justinas Ceponkus[1], Valdas Sablinskas[1], and Pawel Rodziewicz[2] — [1]Faculty of Physics, Vilnius University, Lithuania — [2]Institute of Chemistry, University of Bialystok, Poland

Tetrahydrofuran (THF) is an organic heterocyclic compound, used as an efficient solvent in multifunctional carbon-based nanomaterials e. g. carbon nanotubes. To investigate the interplay between nanomaterial and THF the exact conformation of the solvent should be analyzed in detail. The conformational diversity of the THF molecule is determined by two conformations (C_s envelope, C_2 twisted) with the energy barrier of 1.77 kJ/mol.

In this work matrix isolation infrared absorption spectroscopy was used to study the conformational diversity of the THF molecule at low temperatures. The recorded FT-IR spectra show that at 9 K only one THF conformer is trapped in N_2 matrix, so the pseudorotation is not observed. After heating of the matrix to 25 K additional bands in the IR spectra were observed, what indicates the presence of the second conformer. The *dynamics* of the model THF/N_2 system and the structural rearrangements between its local and global minima have been studied at finite temperature by Car-Parrinello molecular dynamics (CP-MD) simulations.

CPP 28.6 Tue 18:15 Poster B2

Assessment of coarse-grained models of conjugated polymers: Poly(3-hexylthiophene) (P3HT) — •Christoph Scherer and Denis Andrienko — Max Planck Institute for Polymer Research, Mainz, Germany

P3HT is the 'fruit fly' of polymeric organic semiconductors. Its self-assembly into lamellar structures and phase-separation in P3HT:PCBM blends has recently been studied using various computer simulation techniques [1,2,3]. The accuracy of coarse-grained (CG) models was, however, never assessed. Here, (iterative) Boltzmann inversion and force-matching schemes are used to derive interaction potentials for the CG representation of the molecule. The resulting potentials are compared to the ones reported in Refs. [2,3] and are benchmarked against the stability of the crystalline molecular arrangements and the persistence length of a single chain in solvent. The perspective is to include many-body terms into the description of the non-bonded interactions and to implement them into the VOTCA package [4]. The extension of the non-bonded interactions to at least 3-body terms should improve the prediction of the alignment of the polymers as 2-body terms cannot capture the directionality of the Pi-Pi interactions between the thiophene rings of the polymer backbones.

[1] C. Poelking, et al., Adv. Polym. Sci.,265, 139-180, 2014

[2] K. N. Schwarz, et al., Nanoscale, 5, 2017-2027, 2013

[3] E. Jankowski, et al., Macromolecules, 46, 5775-5785, 2013

[4] V. Rühle, et al., J. Chem. Theory Comput., 5, 3211-3223, 2009

CPP 29: Poster: Crystallization, Nucleation, Self Assembly

Time: Tuesday 18:15–21:00 Location: Poster B2

CPP 29.1 Tue 18:15 Poster B2

Non-classical crystallization in the presence of multivalent ions — •Benedikt Sohmen, Andrea Sauter, Fajun Zhang, and Frank Schreiber — Institut für Angewandte Physik - Universität Tübingen, Tübingen, Deutschland

Progress in the understanding of non-classical crystallization pathways of proteins was reported only recently [1]. Here, we present a real-time study of non-classical crystallization of bovine β-lactoglobulin in the presence of $ZnCl_2$ with respect to salt concentration c_s, protein concentration c_p and temperature by optical microscopy. The investigated c_s-c_p-phase diagram can be used as a guide to control and tune the behavior of proteins in solutions. Slightly below a certain salt concentration c* crystals grow in a classical one-step pathway from clear solution. Increasing c_s above c*, up to a certain salt concentration, referred to as pseudo-c**, the crystallization follows a non-classical pathway with a dense phase as intermediate state. The crystals nucleate at the interface between dense and dilute phase. With progressing crystal growth, the dense phase dissolves. Above c**, big aggregates are formed and no crystal growth is observed. The real-time microscopy and x-ray study provides detailed insight into the characteristics of non-classical growth and elucidates the role of the intermediate state.

[1] Sauter et al. J. Am. Chem. Soc. 137,1485-1491, (2015)

CPP 29.2 Tue 18:15 Poster B2

Study on the Crystallization Behavior of Nucleated Polypropylene under Shear at Isothermal Conditions — •Sabine Stockenhuber and Gerhard Eder — Institute of Polymer Science, Johannes Kepler Universität, Linz

Thermoplastic Polymers show big changes in their solidification behavior, orientation and crystallization when they are processed under different conditions. These also alter the mechanical properties of the polymer. An experimental study was performed to show the effect of shear stress, total shear, additive concentration and temperature on crystallinity, orientation and solidification time. The solidification process and therefore the solidification time of the samples without additives was traced by measuring the transmission of light through the sample by an optical system containing a laser, an analyzer and a photodiode detector. The solidification was supposed to be completed when the transmittance was approximately zero. The total shear was controlled manually and obtained by a displacement transducer. The samples from the shear experiments were cut with a microtome perpendicular and parallel to the shear direction. Subsequently, the morphology and orientations were analyzed using polarization microscopy.

CPP 29.3 Tue 18:15 Poster B2

Isothermal and non-isothermal crystallization of polyethylene at large undercooling — •Evgeny Zhuravlev[1], Vadlamudi Madhavi[2], René Androsch[3], and Christoph Schick[1] — [1]University of Rostock, Institute of Physics, Wismarsche Str. 43-45, 18051 Rostock, Germany — [2]ExxonMobil Research & Engineering Company, 1545 Route 22 East, LD 152, Annandale, New Jersey 08801, USA — [3]Martin-Luther-University Halle-Wittenberg, Center for Engineering Sciences, 06099 Halle/S., Germany

The crystallization kinetics of high-density polyethylene and random copolymers of ethylene with up to 16 mol% 1-octene was studied by ultra-fast scanning calorimetry. In order to account for the inherently high crystallization rate of polyethylenes, in non-isothermal and isothermal crystallization experiments cooling rates up to 1,000,000 K/s and crystallization times as short as 10^{-6} s, respectively, were employed. It was possible to supercool the melt of high-density polyethylene down to 57 °C, and the melt of a copolymer with 16 mol% 1-octene down to -33 °C, without prior crystallization. At these temperatures, the characteristic time of the primary crystallization process is of the order of magnitude of 100^{-6} s. Complete vitrification of the liquid would require cooling even faster than 1,000,000 K/s. Compared to the homopolymer, the cooling-rate dependence of the crystallization temperatures and the temperature dependence of the characteristic time of primary crystallization of copolymers both are essentially parallel shifted to lower temperatures, which is suggested being caused by the depression of the equilibrium melting temperature.

CPP 29.4 Tue 18:15 Poster B2

Crystallization of furan-based polyesters — •Andreas Wurm[1], Vasilios Tsanaktis[2], Dimitrios Bikiaris[2], and Christoph Schick[1] — [1]University of Rostock, Inst. of Physics, Germany — [2]Aristotle University of Thessaloniki, Dept. of Chemistry, Greece

Isothermal and non-isothermal crystallization behavior of polymers can be investigated with traditional calorimeters often in a limited temperature region only. This results from the fast crystallization processes on optimal conditions, which appears in most polymers in a few seconds or less. The chip-based fast scanning DSCs allow applying heating and cooling rates of several 1000 K/s, which enables for many polymers to follow crystallization in the whole temperature range between glass transition and melting temperature.

We applied the Mettler Toledo Flash DSC 1 chip calorimeter for investigation of the non-isothermal and isothermal crystallization behavior of different furan-based polyesters from renewable resources (poly(ethylene furanoate) to poly(dodecylene furanoate)). For poly (butylene furanoate) the influence of different nanofillers on the crystallization process is discussed.

CPP 29.5 Tue 18:15 Poster B2

Co-crystallization and Crystal Thickening in Blends of a Double-Crystalline Diblock Copolymer and Corresponding Homopolymers — •Robert Stössel, Tobias Büttner, and Klaus D. Jandt — Chair of Materials Science (CMS), Otto-Schott-Institute for Materials Research, Friedrich Schiller University Jena, Löbdergraben 32, 07743 Jena, Germany

Size and shape of diblock copolymer (DBCP) nanostructures can be varied by blending with homopolymers and/or crystal thickening. In blends of double-crystalline diblock copolymers and crystalline homopolymers co-crystallization can occur. Targeted co-crystallization together with crystal thickening could further extend the range of double-crystalline DBCP nanostructures which was not investigated so far. The aim of the study was to test the hypothesis that the lamellar long period of a double-crystalline polyethylene-block-poly(ethylene oxide) (PE-b-PEO) can be increased by blending with PE and PEO homopolymers as well as by subsequent crystal thickening. Using differential scanning calorimetry, co-crystallization in blends was evaluated by the presence of a single melting endotherm. X-ray scattering experiments showed that co-crystallization can increase the lamellar long period compared to the native PE-b-PEO. Subsequent, annealing experiments revealed crystal thickening of the co-crystals and a further increase of the lamellar long period. Defined co-crystallization and subsequent crystal thickening of double-crystalline DBCP/homopolymer blends can be used to fabricate tailorable nanopatterns for materials science applications in photonics or the biomedical field.

CPP 29.6 Tue 18:15 Poster B2

Real-Time BAM Studies of Cardiolipin Monolayers — •Renko Kensbock, Heiko Ahrens, and Christiane A. Helm — Institute of Physics, University of Greifswald, 17487 Greifswald, Germany

We investigate electrostatic interactions within negatively charged cardiolipin monolayers at the water-air interface with isotherms and real-time Brewster angle microscopy (BAM). A non-monotonic dependence for the LE/LC transition surface pressure on salt concentration (NaCl, KCl) is observed with a maximum at 0.1 mol/l. This is in accordance with calculations taking into account head-group interactions. The calculations consist of an electrostatic contribution (Grahame's equation) and counter-ion binding according to the law of mass action. For salt concentrations above 0.1 mol/l the electrostatic repulsion is predominantly screened, whereas for salt concentrations up to 0.1 mol/l the degree of dissociation increases. The electrostatic interaction also determines the surface area of domains as observed with BAM. Depending on line tension and long range electrostatic repulsion, domain nucleation and growth are differently affected by changes in ionic strength. The observed number of domains, compared at fixed molecular area in the LE/LC coexistence region, shows a similar behavior to that observed with the transition surface pressure - fewest observed domains for the pure water subphase, with an increase in number up to 0.1 mol/l NaCl and thereafter a decrease for 1 mol/l NaCl.

CPP 29.7 Tue 18:15 Poster B2

Modeling of metal cluster growth on hard surfaces — Sven-Jannik Wöhnert[1,2], •Matthias Schwartzkopf[2], Stephan V. Roth[2], and Christian Schroer[2] — [1]Universität Hamburg — [2]Deutsches Elektronen-Synchrotron (DESY)

Sputter deposition is one high-throughput method to install patterned nanostructures on surfaces with high deposition rates. Grazing incidence small-angle X-ray (GISAXS) scattering nowadays delivers a wealth of information during in-situ processes and real-time observations. The geometric model of [1] then allows to extract general cluster parameters to describe the growth of metal clusters on surfaces.

The geometric model of [1] then allows to substract general cluster parameters to describe the growth of metal clusters on surfaces. To gain insight into the specific evolution of cluster growth, we investigated cluster formation during sputter deposition at different temperatures on various hard surfaces in order to discover dependencies and relations on atomic level.

Therefore, we present a phenomenological Monte-Carlo simulation comparing cluster parameters with the results of the GISAXS measurements. We provide information about the dependencies of surface diffusion, nucleation and cluster interaction on the cluster evolution.

[1] Schwartzkopf et al., Nanoscale 5, 5053 (2013)

CPP 29.8 Tue 18:15 Poster B2

A tensor-based model for the interaction of charged Janus particles — •Reint Hieronimus and Andreas Heuer — Westfälische Wilhelms-Universität Münster, Institut für physikalische Chemie, Corrensstrasse 30, 48149 Münster, Germany

We analyse the interaction of charged Janus spheres, including screening effects. The explicit interaction is mapped via a least square method on a variable number n of systematically generated tensors that reflect the angular dependence of the potential. For $n = 2$ we show that the interaction is equivalent to a model previosly described by Erdmann, Kröger and Hess[1]. Interestingly, this mapping is not able to capture the subtleties of the interaction for small screening lengths. Rather, a larger number of tensors has to be used. We obtained cluster structures up to the size of 13 particles for $n = 2, 36$ and screening lengths $\kappa^{-1} = 0.1, 1.0$ that we analysed to discuss the influence of the screening length. The cluster structures are also compared to results for an explicit electrostatic potential[2] and for the DLVO theory[3].

[1] T. Erdmann, M. Kröger, S. Hess, Phys. Rev. E 2003, 67, 041209

[2] L. Hong, A. Cacciuto, E. Luijten, S. Granick, Nano Letters 2006, 6, 2510–2514

[3] J. de Graaf, N. Boon, M. Dijkstra, R. van Roij, J. Chem. Phys., 2012, 137, 104910

CPP 30: Poster: Organic Electronics and Photovoltaics

Time: Tuesday 18:15–21:00 Location: Poster B2

CPP 30.1 Tue 18:15 Poster B2

Microstructure of donor-acceptor conjugated polymer blends and annealing induced nano-aggregation observed by two-dimensional polarization fluorescence microscopy — •Daniela Täuber[1], Yuxi Tian[1], Yuxin Xia[2], Olle Inganäs[2], and Ivan Scheblykin[1] — [1]Chemical Physics, Lund University, Lund, Sweden — [2]Biomolecular and Organic Electronics, Linköping University, Linköping, Sweden

Polymer-polymer bulk heterojunction solar cell devices combine solar energy harvesting with the fortune of polymer materials, which enable easy and inexpensive processing and flexibility of the material.

Their performance crucially depends on the organization of the conjugated polymer molecules. Studying blends of TQ1 and N2200 spincast from solution with two-dimensional polarization fluorescence microscopy we observe concentration dependent microstructures. Comparing polarization parameters from films as prepared with films annealed at 120°C, we find modifications pointing to enhanced nano-aggregation of the annealed polymer blend. These changes agree with modifications seen in fluorescence and absorption spectra and in fluorescence lifetime measurements.

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

CPP 30.2 Tue 18:15 Poster B2

Conformational preferences of conjugated benzothiadiazole-cored oligomers: the impact of through-space interactions — •Deyan Raychev[1,2], Olga Guskova[1,2], and Jens-Uwe Sommer[1,2,3] — [1]Dresden Center for Computational Materials Science, TU Dresden — [2]IPF Dresden — [3]Institute of Theoretical Physics, TU Dresden

Symmetrical benzothiadiazole-cored oligomers with thiophene or furan rings are widely used in experiments as structural blocks for organic electronics. Along with chemical composition, the molecular conformation plays a crucial role in crystal packing/self-assembly of these building moduli in thin films. In this work, we examine the conformational preferences analyzing possible through-space interactions (S...N, O...N, S...H, O...H), steric repulsion, electrostatics and donor/acceptor orbital interactions for a series of benzothiadiazole-based conjugated oligomers using DFT calculations (with different functionals and basis sets and taking into account the effects of the medium) and NCI procedure [1].

The financial support from ESF Young Investigators Group CoSiMa (TU Dresden) is highly appreciated.

[1] J. Contreras-García et al. J. Chem. Theory Comput. 7 (3), 625-632 (2011).

CPP 30.3 Tue 18:15 Poster B2

Influence of conformations in DPP-TH based molecular system on electronic structure and charge transport properties — Maria V. Makarova[1], Sergey G. Semenov[2], and •Olga Guskova[1,3] — [1]IPF Dresden, Dresden, Germany — [2]Petersburg Nuclear Physics Institute, National Research Centre "Kurchatov Institute", Gatchina, Russia — [3]Dresden Center for Computational Materials Science (DCMS), TU Dresden, Dresden, Germany

Such phenomenon as stereoisomerism can strongly influence on physical and chemical processes in molecular systems. In the present work, the role of conformational changes on charge transport process in diketopyrrolopyrrole-thiophene (DPP-TH) molecular system was theoretically investigated. Quantum chemical calculations of relative and reorganization energies, ionization potentials, electron affinities and intermolecular couplings were performed for two TH2-DPP-TH2 conformers. Calculations were carried out by M06-2X/cc-pVDZ method using GAUSSIAN09. Crystal structure predictions (Monte Carlo method) were performed using BIOVIA Materials Studio 8.0.

CPP 30.4 Tue 18:15 Poster B2

Manipulation and controlling the strength of the interfacial polarisation in OLED devices by doping — •Lars Jäger, Tobias D. Schmidt, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Most of the used electron transporting materials in organic light emitting diodes are known to be polar. This property modifies the internal electric field distribution of the device and therefore enables an earlier flat band condition for the hole transporting side, leading to improved charge injection. Recently the interfacial polarisation has been investigated with regard to different materials and degradation effects, however, so far the influence of doping has never been looked at. Here we focus on the behavior in the case of doping of the polar electron transporting layer tris-(8-hydroxyquinolate) aluminum (Alq_3) with the hole transporting material 4,4'-bis[N-(1-naphthyl)-N-phenylamino]-biphenyl (NPB). By evaluating impedance spectroscopy data we can show that the limiting parameter is not the effective Alq_3 thickness. In fact the built up of the polarisation reaches a maximum for a 50% blend. Taking the permanent dipole moments of the molecules into account, an increasing contribution was found for a decreasing Alq_3 amount in the blend. This fact can be explained by a sterically mechanism in addition to the minimization of the dipole-dipole interaction.

CPP 30.5 Tue 18:15 Poster B2

Printing High Efficiency Solar Cells — •Dan Yang and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Printing techniques hold a promising future for thin organic films. The realization of fast, low-cost and large areas manufacture lies within reach. In our work, we combine the printing technique with high power conversion efficiency (PCE) polymers to prepare organic solar cells. In the past few years, a new state-of-the-art low bandgap polymer with PCEs exceeding 7%, polythieno [3, 4-b]-thiophene-co-benzodithiophene (PTB7), has been developed as one of the most promising donor materials for organic solar cells. So far, research focused on PTB7 films prepared via spin coating to make such solar cells. In contrast, we prepare solar cells (PTB7 as donor) with printing the active layers. We measure the device function via I-V curves. In order to understand the influence of printing, we investigate the morphology of the active layers with GISAXS and the crystal orientation with GIWAXS.

CPP 30.6 Tue 18:15 Poster B2

Degradation processes in high-efficiency polymer solar cells — •Christoph Senfter, Franziska Löhrer, Christoph Schaffer, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

The application of polymers as active material in solar cells has several advantages over conventional silicon solar cells. Organic materials are typically cheap in production, flexible and lightweight, but their efficiencies and long term stabilities are far below the ones of their inorganic counterparts. In the last years, research has been focusing on the identification of new high-efficiency polymers like PTB7-Th with reported efficiencies surpassing 10 % in combination with PC71BM. However, little is known about the long-term stability of this polymer and its blends. Photo-oxidation and morphological changes of the active layer are two main aging processes, which lower the cell performance over time. To learn more about the degradation process, we investigate changes of the polymer under illumination using FT-IR spectroscopy. Additional investigation methods include optical characterization via UV/Vis and PL as well as morphological characterization using X-ray diffraction methods. The change in cell performance is probed by applying IV-measurements.

CPP 30.7 Tue 18:15 Poster B2

Hole mobility in bulk P3HT determined from first principles — •Andreas Lücke[1], Frank Ortmann[2], Simone Sanna[1], Eva Rauls[1], Uwe Gerstmann[1], and Wolf Gero Schmidt[1] — [1]Lehrstuhl für Theoretische Physik, Universität Paderborn, 33095 Paderborn, Germany — [2]Institute for Materials Science and Dresden Center for Computational Materials Science, Technische Universität Dresden, Germany

The temperature-dependent hole mobility for ideal Poly(3-hexylthiophene) (P3HT) crystals is calculated ab initio and compared with experimental data. Thereby the electronic structure as well as phonon frequencies and electron-phonon coupling constants are obtained from density functional theory. The P3HT transport properties are dominated by polarons due to the strong coupling between the charge carriers and the vibrating lattice. By providing a limit for ideal

P3HT crystals, our results allow for separating the polaron effects from disorder contributions onto the temperature dependent mobility. Furthermore a detailed analysis of important phonon modes is given that illustrates the polaron effects microscopically.

CPP 30.8 Tue 18:15 Poster B2

Investigation of the donor-acceptor coupling strength in DBP:C_{70} solar cells — •Thomas Zechel, Theresa Linderl, Thomas Lampe, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86159 Augsburg

The strength of the donor (D) acceptor (A) interaction can have an influence on the open circuit Voltage (V_{OC}) in organic solar cells as demonstrated by Vandewal *et al.* [1]. Here it is shown that the strength of the D-A interaction in Tetraphenyldibenzoperiflanthen(DBP):Fulleren C_{70} planar mixed hetero junction (PM-HJ) solar cells decreases with decreasing the amount of DBP in the mixed layer. However, no significant changes in V_{OC} for this D-A pairing can be observed. The coupling strength is obtained from electroluminescence (EL) and external quantum efficiency spectra of working devices. Temperature dependent EL measurements reveal two charge transfer peaks with different temperature dependence. At the same time the current voltage characteristics of the different devices show that only a small amount of DBP is necessary for efficient charge separation.

[1] Vandewal, K. *et al.*, Physical Review B, **2010**, *81*, 125204

CPP 30.9 Tue 18:15 Poster B2

Light-coupling and light trapping in periodically structured thin-film solar cells — Thomas Pfadler and •Lukas Schmidt-Mende — Universität Konstanz

Periodically structured TiO2 electrodes are introduced to thin-film photovoltaics to tackle the typically partial light absorption. Arising consequences on light management in such thin-film solar cells are elucidated. Wavelength-scale patterns are transferred to the electron-selective TiO2 bottom electrodes via direct laser interference patterning. In the main absorption region of the employed photoactive materials, the efficiency of the structure-induced light in-coupling is spectroscopically shown to be determined by the refractive index n(active material) with respect to n(TiO2). Beside the elucidation of light in-coupling in the main absorption region of the photoactive material, structure-induced light-trapping effects targeting at a resonant enhancement of the very weak tail-state absorption present in polymer:fullerene BHJ solar cells are additionally investigated. The presented approach paves the way to potentially close the gap between net optical and electric band gap of organic solar cells, which is stated as an intrinsic energy loss mechanism in donor-acceptor systems. Furthermore, fully vectorial electromagnetic simulations using the Discontinuous Galerkin Time Domain method were performed to obtain time-averaged Poynting vectors along with spatially resolved dependencies of the power loss densities. The simulations underline the experimental findings and further outline the tuneability of the absorption resonances towards arbitrary wavelength regions.

CPP 30.10 Tue 18:15 Poster B2

Disorder effects on Charge Transport in Rubrene Crystals — •Michel Panhans[1], Desanka Boskovic[2], Pablo Ordejón[2,3], and Frank Ortmann[1] — [1]Institute for Material Science and Dresden Center for Computational Material Science, Technische Universität Dresden, 01062 Dresden, DE — [2]ICN2 - Institut Catala de Nanociencia i Nanotecnologia, 08193 Bellaterra, ES — [3]CSIC - Consejo Superior de Investigaciones Cientificas, 08193 Bellaterra, ES

The understanding of charge transport in small-molecule organic semiconductors challenges both experimental and theoretical approaches since many 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 present a charge transport approach based on ab initio calculations of all relevant parameters of the small molecules that tackles electron-phonon interactions both quantum-mechanically and semi-classically and includes disorder effects by suitable real space models.

The p-type charge transport in rubrene single-crystals FET's serves as a test case that provides a valuable reference for comparison with our charge transport simulations of rubrene crystals. Based on the present theory we studied band-like transport and phonon assisted hopping transport in the presence of two different sources of disorder and compared them quantitatively to existing experimental data. The analysis of both models illustrates important aspects of transport mechanisms occurring in organic small-molecule semiconductors.

CPP 30.11 Tue 18:15 Poster B2

Columnar axial orientation of discotic liquid crystals in nanoporous solids — •Kathrin Sentker, Katrin Knopp, and Patrick Huber — Institut für Werkstoffphysik und -technologie, Technische Universität Hamburg-Harburg

The columnar axial orientation of discotic liquid crystals (DLC) in nanoporous silica or alumina membranes provides a high electrical conductivity along the pore axis, which is important for their applications in e.g. photovoltaic devices. The optical birefringence of the DLCs is a measure of their orientational order. In contrast to a radial orientation an axial orientation causes a negative birefringence. We successfully reproduced the experimental results of Calus et al. [1], showing that 11-hexakis(hexyloxy)triphenylene DLCs embedded in an untreated alumina membrane exhibit positive birefringence, hence a radial orientation. In order to achieve axial orientation we are going to chemically modify the membranes from hydrophilic to hydrophobic. Additionally, we are going to perform measurements with coronene-based DLCs as suggested by Duran et al. [2], supplemented by X-ray diffraction experiments to probe the translational order.

[1] Sylwia Calus, Andriy V. Kityk, Patrick Huber, Microporous and Mesoporous Materials 197 (2014)

[2] Hatice Duran et al., ACS Nano 6, 11 (2012)

CPP 30.12 Tue 18:15 Poster B2

Energy losses in DIP/PDIR-CN_2 based solar cells. — •Eduard Meister[1], Theresa Linderl[1], Stefan Schmidt[1], Thomas Zechel[1], Paul Beyer[2], Andreas Opitz[2], Valentina Belova[3], Alexander Hinderhofer[3], Frank Schreiber[3], and Wolfgang Brütting[1] — [1]Institut für Physik, Universität Augsburg, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Germany — [3]Institut für Angewandte Physik, Universität Tübingen, Germany

Perylene derivatives are widely used in organic electronics. Depending on the substitution at both ends of the molecular core, either donor- or acceptor-type behaviour is obtained. In this contribution we used diindenoperylene (DIP) as donor and N,N'-bis-(2-ethylhexyl)-1,7-dicyanoperylene-3,4:9,10-bis(dicarboxyimide) (PDIR-CN_2) as acceptor and prepared donor/acceptor (D/A) solar cells with two different architectures: planar hetero junction (PHJ) and planar mixed hetero junction (PM-HJ). The j-V measurements displayed that the open circuit voltage V_{OC} of both architectures, PM-HJ and PHJ, is equal, where the short circuit current density j_{SC} as well as the efficiency for the PM-HJ cell is lower than for its PHJ pendant. In addition we determined from electroluminescence (EL) measurement two radiative CT states and from incident photon-to-current efficiency (IPCE) experiment at least four CT states. Taken as a whole, this D/A combination yields very low efficiency, most likely due to a strong interaction between DIP and PDIR-CN_2 accompanied by very high non-radiative energy losses detected with EL and IPCE measurements.

CPP 30.13 Tue 18:15 Poster B2

In situ polymerized insoluble semiconducting polymers for application in organic solar cells — •Jenny Lebert, Anna Sanina, Eva Kratzer, and Eva M. Herzig — Technische Universität München, Munich School of Engineering, Lichtenbergstr. 4, 85748 Garching

Organic semiconducting materials can be applied in optoelectronic devices such as organic light-emitting diodes and organic solar cells. The polymers employed usually exhibit a conjugated backbone of varying complexity which is equipped with insulating, alkyl side chains to make them processable from solution. While nowadays lab scale organic solar cells can easily perform at efficiencies above ten percent, they still suffer from fast degradation induced amongst others by external impacts such as water, oxygen and UV light. In situ polymerization offers the possibility to process polymers from solution without the need for solubilizing side chains. Thereby the amount of electrically insulating molecular parts in the film are reduced to a minimum. Moreover, the simplified chemical structure of the polymers leads to a higher stability. In this work, in situ polymerized polythiophene thin films are investigated in terms of their stability in organic solar cells. For this purpose, differently post-treated films are analyzed regarding their morphology, conductivity and optoelectronic properties.

CPP 30.14 Tue 18:15 Poster B2

Investigating the photoactive layer morphology of printed thin films for organic solar cells — •Oliver Filonik[1,2], Stephan Pröller[1], Peter Müller-Buschbaum[3], and Eva M. Herzig[1]

— [1]Technische Universität München, Munich School of Engineering, 85748 Garching, Germany — [2]Technische Universität München, LS Erneuerbare und Nachhaltige Energiesysteme, 85748 Garching, Germany — [3]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Organic solar cells yield numerous advantages including flexibility, low material costs, and independence on rare resources. In particular, solution based processability enables fabrication techniques like printing, which is up-scalable to large area photovoltaics production in industrial processes. The photoactive layer morphology, consisting of a donor and acceptor material blend, is of utmost importance for the performance of the device due to its impact on the exciton generation, exciton separation and charge carrier transport in the device. Therefore, a deeper understanding of the parameters influencing the active layer's morphology is crucial.

Using a slot die coater, we print organic thin films used as the photoactive layer of an organic solar cell. We investigate the processing parameters as well as external influences on the film morphology in order to obtain insight into the crucial processing parameters for the photoactive layer. With this knowledge, we are able to optimize the production process of organic solar cells.

CPP 30.15 Tue 18:15 Poster B2

Diffusion of p-type Dopants in Organic Semiconductors — •Dongxiang Wang[1,2], Lars Müller[2,3,4], Sebastian Beck[2,4], Robert Lovrincic[2,3], Uli Lemmer[1,2], and Wolfgang Kowalskty[2,3] — [1]KSOP, Karlsruhe Institute of Technology, Germany — [2]InnovationLab, Heidelberg, Germany — [3]IHF, TU Braunschweig, Germany — [4]KIP, Heidelberg University, Germany

Molecular doping of organic semiconductors is routinely applied in various devices such as organic light emitting diodes. Nevertheless, issues like the diffusion of dopants are still not solved for many material combinations. In this work, we investigate if this diffusion can be controlled to improve device performance. The starting device is a diode with two gold electrodes evaporated onto a substrate and the organic semiconductor material (P3HT) doped with certain p-type dopants such as F4TCNQ. Chlorobenzene is used as solvent for the solution-fabricating process. To get a general understanding of how dopant diffusion can be controlled, we start with an application of an electric field. Conductivity measurements as well as IR and UV-Vis spectroscopy are performed for the investigation. We show that the dopant distribution in the matrix material can indeed be controlled via an applied electric field. We will discuss how this effect can be utilized to improve the performance of an organic field effect transistor.

CPP 30.16 Tue 18:15 Poster B2

Influence of crosslinking on charge carrier mobility in PF2/6-derivatives — •Frank-Julian Kahle[1], Irene Bauer[2], Anna Köhler[1], and Peter Strohriegl[2] — [1]Department of Physics, University of Bayreuth, Germany — [2]Department of Chemistry, University of Bayreuth, Germany

Cross-linking provides a good means to fabricate optoelectronic devices with multiple layers via solution processing. In the current work, a series of especially synthesized PF2/6 derivatives with different fractions of cross-linkable acrylate groups is investigated. Spectroscopic characterization and mobility measurements are carried out to assess the influence of introducing acrylate groups and crosslinking on material performance. For the regime of low to medium charge carrier density, relevant for OLEDs and OPVs, we used a novel technique based on the injection of charge carriers from the electrodes of an optoelectronic device: MIS-CELIV. This technique allows for the selective measurement of electron or hole mobility. By comparing crosslinked samples with pure PF2/6 as reference, we could show that the crosslinking process itself does not significantly influence hole mobility in the investigated system. An observed reduction of about one order of magnitude is attributed to structural differences caused by the introduction of acrylate groups. Furthermore, it turned out that the crosslinking process may be solely triggered by thermal activation and UV-illumination without the need of any photoinitiator, still achieving a densely linked network. This is of special interest as we have seen that a larger amount of photoinitiator may introduce traps for charge carrier transport.

CPP 30.17 Tue 18:15 Poster B2

Organic heterojunctions: Contact-induced molecular reorientation, interface states, and charge re-distribution — •Paul Beyer[1], Tino Meisel[1], Alexander Generalov[2], Ana Sofia Anselmo[3], and Andreas Opitz[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Germany — [2]Maxlab, Lund University, Sweden — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

Different relative molecular orientations at organic-organic heterointerfaces dictate the orbital overlap between neighboring molecules, as well as electronic and structural properties, which are crucial for organic electronic devices. In order to access these properties we utilize a multi-technique approach, consisting of I/V measurements, absorption and photoelectron spectroscopy.

As a donor/acceptor combination, we chose two perylene derivatives: diindenoperylene (DIP) and functionalized perylene alkyldiimide with cyano groups (PDIR-CN$_2$). The usage of different substrates allows us to tune the molecular orientation inside the grown thin films. We investigated different devices with relevant architectures – planar heterojunctions (PHJ) and planar mixed heterojunctions (PM-HJ).

From absorption measurements, we observed blend exclusive features, proving the creation of new charge transfer states, specifically charge transfer excitons. Depending on the molecular orientation and, thus, the interface geometries, we found clear changes in ionization energies compared to the pristine materials, stemming from differences in energy level alignment.

CPP 30.18 Tue 18:15 Poster B2

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 (BIMF)

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 PCPDTBT-PCBM blends with a resolution of 200fs. The charge transfer is measured by monitoring the transient absorption of the polymer cation after excitation. We find no change in transfer dynamics upon cooling to 12K within our temporal resolution. This result suggests that initial charge transfer lacks thermal activation.

CPP 30.19 Tue 18:15 Poster B2

Preparation and Characterization of Ionic Transistors — •Martin Gebhardt[1,2], Lars Müller[1,2], Robert Lovrincic[1,2], and Wolfgang Kowalsky[1,2] — [1]Institute for High-Frequency Technology, TU Braunschweig, Germany — [2]InnovationLab GmbH, Heidelberg, Germany

In contrast to electron based transistors, most transmissions inside the human body depend on ions and molecules. To have an interface between electronics and the biological world, ion bipolar junction transistors (IBJT) were studied. The built IBJTs consist of two organic bipolar membranes and an electrolyte in between. When applying a voltage to the base of the IBJT, ions are injected into the junction and a current of opposite polarized ions flows from emitter to collector. In cut-off mode the junction is depleted of the base-ions and the current of the emitter-collector-ions stops. We present the fabrication of IBJTs and discuss the performance of them with respect to changes of the geometry.

CPP 30.20 Tue 18:15 Poster B2

Theoretical core level XPS and NEXAFS investigations of the C$_{60}$ derivative PCBM: the influence of oxygen adsorption — •Iulia Emilia Brumboiu[1], Leif Ericsson[2], Rickard Hansson[2], Ellen Moons[2], Olle Eriksson[1], and Barbara Brena[1] — [1]Department of Physics and Astronomy, Uppsala University, SE-75120 Uppsala, Sweden — [2]Department of Engineering and Physics, Karlstad University, SE-65188 Karlstad, Sweden

In recent years, organic photovoltaics (OPVs) have been developing as an alternative to silicon solar cells. Some of the advantages of OPVs are device flexibility, low production cost and low environmental impact. Device efficiencies have recently reached 10%, a limit that makes OPVs competitive on the market. One of the main issues that still needs to be resolved is the stability of the cells. Both the electron donor (organic polymer) and the electron acceptor (fullerene derivative) have been shown to undergo degradation during device functioning. We have addressed in this study one of the possible degradation mechanisms involving the electron acceptor PC$_{60}$BM . Specifically, we have studied by means of density functional theory (DFT) the possible final products of oxygen adsorption on the C$_{60}$ cage. Several configurations of PC$_{60}$BM with oxygen have been analysed from the point of view of the molecular structure, of the O 1s near edge x-ray absorption fine structure (NEXAFS) and of the x-ray photoelectron spectrum (XPS). We show that a joint O 1s XPS and NEXAFS study could provide insight into both the nature of the adsorbate (atomic or molecular oxygen) and the bonding configuration.

CPP 30.21 Tue 18:15 Poster B2

Chemical doping of semiconduting donor-acceptor polymers: a DFT study of the charge transfer — •Florian Günther[1,2], Anton Kiriy[3], Sibylle Gemming[1,4], and Gotthard Seifert[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Leibniz-Institut für Polymerforschung Dresden,Dresden,Germany — [3]Institute of Physical Chemistry and Electrochemistry, Dresden University of Technology, Dresden, Germany — [4]Institute of Physics, Technical University Chemnitz, Germany

Donor-acceptor (DA) polymers have recently been considered as promising candidates for novel organic electronics such as organic field effect transistors. Combining these systems with organic molecules having high electron affinity (low ionisation potential) leads to a charge transfer, and thus to doping of the organic semiconductor.

In this study, we theoretically evaluate the charge transfer between DA model compounds as Diketopyrrolopyrrole-dithienylthieno[3,2-b]thiophene (DPP-TT) and p-dopant molecules as tetrafluorotetracyanoquinodimethane (F4-TCNQ) based on density functional theory (DFT) calculations. Furthermore, different structural formations are under consideration in order to obtain most stable configurations.

Interestingly, we observe in the lowest energy complex, the dopant molecule is located quite closely to the acceptor unit of the polymer (DPP) where the charge transfer process proceeds to the lowest extend.

CPP 30.22 Tue 18:15 Poster B2

Molecular doping of conjugated polymers with the strong Lewis acid tris(pentafluorophenyl)borane — •Malavika Arvind[1], Patrick Pingel[2], and Dieter Neher[1] — [1]University of Potsdam, Soft Matter Physics, Potsdam, Germany — [2]Fraunhofer Institute for Applied Polymer Research, Potsdam, Germany

In the past years, conjugated polymers have acquired a great deal of interest as semiconductors in electronic devices due to their attractive properties such as mechanical flexibility and easy processability. Efficient charge transport through the semiconductor layers is a crucial requirement in electronic devices. Molecular doping provides an easy means of tuning and improving the transport properties of these materials. In this work, doping of the conjugated polymer poly(3-hexylthiophene) (P3HT) with the strong Lewis acid tris(pentafluorohenyl)borane (BCF) is studied using UV-Vis spectroscopy and conductivity measurements. By assigning the sub-band gap signals observed in the optical spectra of the doped solutions and layers to the known spectral signatures of the charged species in P3HT, the nature of charged species formed, the predominant mechanism of charge transfer between the dopant and polymer, and the doping efficiency is analyzed. While charge transfer is rather inefficient in solution, ca. 50 % of the employed dopant molecules undergo integer charge transfer with the polymer in solid state. Comparison with the well-known acceptor F4TCNQ reveals important differences with regard to the degree of ionization and the quality of the doped layer, which we assign to the better solubility and bulky structure of BCF.

CPP 30.23 Tue 18:15 Poster B2

Investigation and tuning of merocyanine dye thin films on ultra-flat substrates — •Thorsten Limböck, Dirk Hertel, and Klaus Meerholz — Institut für Physikalische Chemie, Universität zu Köln, Luxemburger Str. 116, 50939 Köln

Organic solar cells provide a low cost, yet, due to their thin film architecture, versatile alternative to the established silicon-based solar cells. One of the main challenges of organic photovoltaics is the relatively modest power conversion efficiency. To improve on the efficiency, the morphology of each individual layer has to be tuned in order to optimize the absorption, charge generation and charge transport. To investigate the morphology of dipolar molecules a merocyanine dye layer is grown in a controlled environment via vacuum deposition on ultra-flat substrates graphite and mica in comparison to conventional organic photovoltaic electrode materials, such as ITO, MoO$_3$ or PEDOT. The morphologic behavior of its ordered growth and the changes therein for a variation of different parameters, such as layer thickness, evaporation rate and substrate temperature are investigated via atomic force microscopy and kelvin probe force microscopy. The achievable tuning range stretches from an amorphous form to large scale highly ordered layers with island sizes of several hundred μm^2. To investigate electric transport properties, organic field-effect transistors are build, which contain engineered layers of the merocyanine dye. The investigation is extended to other merocyanines having a lower polarity.

CPP 30.24 Tue 18:15 Poster B2

Charge transfer energies for organic donor acceptor pairs — •Janna Elisabeth Rückert[1,2], Sebastian Schellhammer[1,2,3], Gianaurelio Cuniberti[1,2,3], and Frank Ortmann[1,2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Technische Universität Dresden, 01062 Dresden, Germany — [2]Dresden Center for Computational Materials Science, Technische Universität Dresden, 01062 Dresden, Germany — [3]Center for Advancing Electronics Dresden, Technische Universität Dresden, 01062 Dresden, Germany

Organic solar cells depend heavily on the energetics close to the donor acceptor interface. We theoretically investigate the excitations of donor acceptor pairs based on C60 molecules and varying donor species. By means of time-dependent density functional theory simulations, we analyze the charge transfer energy and the absorption strength. We investigate the influence of the geometric configuration on the excitation energy and on the oscillator strength and find that the configuration of the molecular dimer has a strong impact on the absorption strength while the CT energy is weakly affected.

CPP 30.25 Tue 18:15 Poster B2

Effect of the donor orientation on the V_{OC} losses in small molecule organic bilayer solar cells. — •Steffen Roland[1], Niva Ran[2], Thuc-Quyen Nguyen[2], and Dieter Neher[1] — [1]University of Potsdam, Institute of Physics and Astronomie, Potsdam, Germany — [2]University of California Santa Barbara, Center for Advanced Organic Photovoltaics, USA

Bilayer solar cells based on the donor molecule p-SIDT(FBTTh$_2$)$_2$ and the acceptor molecule C_{60} show a significant difference in the V_{OC} of about 110 mV depending on whether the donor molecule exhibit an edge-on or face-on orientation. Here, we perform a detailed analysis of the losses determining the V_{OC} in these devices. By analyzing EQE and EL spectra related to the CT state, we find the effect of donor orientation on the CT energy not to be sufficient to explain the full V_{OC} difference. In accordance to this, we see almost no change of the HOMO energy in dependence of the orientation of the donor molecules. On the other hand, the absolute EL efficiency is significantly reduced in the bilayer cell with the edge-on oriented donor compared to the cell with face-on oriented donor molecules, pointing to increased non-radiative CT recombination.This shows that the molecular orientation can play a key role in determining non-radiative V_{OC} losses in organic photovoltaics.

CPP 30.26 Tue 18:15 Poster B2

Spatial Orientation and Order of Structure-Defining Subunits in Thin Films of a High Electron Mobility n-Type Copolymer (P(NDI2OD-T2)) as Studied by Infrared Transition Moment Orientational Analysis (IR-TMOA) — •Arthur Markus Anton[1], Robert Steyrleuthner[2,3], Wilhelm Kossack[1], Falk Frenzel[1], Dieter Neher[2], and Friedrich Kremer[1] — [1]Universität Leipzig, Institut für Experimentelle Physik I, Leipzig, Germany — [2]Universität Potsdam, Intitut für Physik und astronomie, Potsdam, Germany — [3]Freie Universität Berlin, Fachberecih Physik, Berlin, Germany

In order to investigate the molecular order in thin layers of P(NDI2OD-T2) the method of infrared transition moment orientational analysis (IR–TMOA), is employed. Structure-specific vibrational bands are analyzed in dependence on polarization *and* inclination of the sample film with respect to the optical axis. By means of IR specificity we deduce the molecular order parameter tensor for the respective moieties with regard to the sample coordinate system and determine independently the orientation and order of atomistic planes defined through the naphthalenediimide (NDI) and bithiophene (T2) units relative to the substrate, and hence, relative to each other. We observe that the polymer backbones in a 150 nm-thick film exhibit a pronounced in-plane anisotropy proving self-aggregated long range order, even though the sample is spin-coated from solution. For μm-thick films the anisotropy vanishes while the inclination of the NDI unit remains basically unaffected. [Anton et al., *J. Am. Chem. Soc.* **137** (2015) 6034]

CPP 30.27 Tue 18:15 Poster B2

Charge Transport in Donor-Acceptor Polymeric Systems under Electric Fields — •Anja Förster[1,2], Florian Günther[1,2,3], Sibylle Gemming[2,3], and Gotthard Seifert[1,2] — [1]Theoretical Chemistry, TU Dresden, Dresden, Germany — [2]Center for Advancing Electronics Dresden (cfaed), Dresden, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Printable and foldable organic transistors are meant to revolutionize electronic applications. However, in comparison to their silicon counterparts their performance is currently still lacking. Thus, we investigate possible options of improving the charge transport in donor-acceptor polymers via DFT calculations.

The first focus point is the influence of gate-induced electric fields. Here, we concentrate on the preferable orientation of diketopyrrolopyrrole-dithienylthieno[3,2-b]thiophene (DPPT-TT) inside the transistor. We further analyze if source-drain induced electric fields have to be taken into consideration when describing the transport in DPPT-TT. We show that strong electric fields are required to yield significant changes in the transport properties.

A second option to improve the charge transport process is to functionalize DPPT-TT via fluoroalkyl chains. Here, the fluorine atoms introduce dipole fields and electron withdrawing sites. We concentrate on finding the composition of fluoroalkyl chains that yields the highest improvement in the charge transport process.

CPP 30.28 Tue 18:15 Poster B2

Nucleation of C70-aggregates on pentacene thin films for nanostructuring organic interfaces — •Janina Roemer, Simon Noever, Stefan Fischer, Clemens Liewald, and Bert Nickel — Ludwig-Maximilians-Universität, Fakultät für Physik, München, Germany

Organic heterojunctions with well defined, nanostructured interfaces are desired for the investigation of interface effects. We use molecular beam deposition to create model-like, nanoscale interfaces by self-assembly of C70-aggregates on pentacene thin films. Size and distribution of these fullerene-islands can be tuned by the choice of evaporation rate and sample temperature.

An accompanying growth study utilizing x-ray Bragg scattering in reflection geometry, grazing incidence diffraction and atomic force microscopy on pentacene-C70 bilayer systems gives insight into the basic growth mechanism of the fullerene. In combination with in-situ measurements of thin film transistor characteristics during growth of the active layer, this allows us to correlate electronic effects, such as charging phenomena at the interface, with nanomorphology.

In future measurements we plan to apply photoresponse microscopy to study charge transfer at the pentacene-C70 heterojunction.

CPP 30.29 Tue 18:15 Poster B2

Rational design of thermally activated delayed fluorescence materials: The competition between internal conversion and non-radiative decay processes — •Paul Kleine[1], Ramunas Lygaitis[1,2], Ludwig Popp[1], Florian Wüst[1], Olaf Zeika[1], Simone Lenk[1], Reinhard Scholz[1], and Sebastian Reineke[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, Germany — [2]Department of Polymer Chemistry and Technology, Kaunas University of Technology, Lithuania

Under electroluminescence operation, about 75 % of the excitons formed in organic light-emitting diodes (OLEDs) come to life as triplet states. While phosphorescent OLEDs make use of rare metal complexes to increase triplet harvesting, the stability and substantial efficiency roll-off at higher current densities remain open issues. Although there has been an amazing progress in thermally activated delayed fluorescent (TADF) emitters, the overall understanding of the TADF unlocking molecular properties to upconvert tripet states is still in its infancy and the fundamental properties to tackle are still under debate. To increase the internal quantum efficiency of TADF materials, the competition between internal conversion, radiative, and non-radiative rates decides over good and bad emitter molecules. In this talk, we will present our recent efforts in the understanding of the basic concepts of TADF mechanism. Rational design and subsequent photophysical investigations of new types of TADF materials confirm the competition between multiple internal transfer rates which open the path to improved design structures for TADF in general.

CPP 30.30 Tue 18:15 Poster B2

First Solution-Processed White OLEDs Exhibiting TTA Delayed Fluorescence — •Merve Welnhofer, Christian Töpel, Anne Köhnen, Jürgen Schelter, Dirk Hertel, and Klaus Meerholz — Department of Chemistry, University of Cologne, Luxemburger Str. 116, 50939 Cologne, Germany

In past decades organic light emitting diodes (OLED) have drawn much attention due to their superior properties over the established lighting and display technologies. Although OLEDs have already found their way into commercial products, a major drawback is loss of three quarters of electrically generated excitons due to radiationless relaxation from triplet excitons. One approach to solve is to collect the triplet excitons by energy transfer between two triplet excitons to generate a singlet exciton relax radiatively by means of triplet-triplet annihilation (TTA). So far many organic molecules revealing TTA with different emission wavelengths are reported however none of them was suitable for solution processable OLEDs. We report on the first solution processed TTA type multilayer OLEDs containing oxetane functionalized (crosslinkable) anthracene derivatives that are emitting in the blue, green, yellow and red wavelength region. To our knowledge these devices are the first fully solution-processed OLEDs revealing TTA delayed fluorescence (DF). Additionally, we used these materials to fabricate the first solution-processed white DF-OLEDs.

CPP 30.31 Tue 18:15 Poster B2

Thermally activated delayed fluorescence (TADF) in organic light emitting devices (OLEDs) utilizing carbazol-donor-benzofluoride-acceptor complexes — •Ludwig Popp[1], Reinhard Scholz[1], Paul Kleine[1], Ramunas Lygaitis[1,2], Florian Wüst[1], Eni Dodbiba[1], Simone Lenk[1], and Sebastian Reineke[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, Germany — [2]Department of Organic Technology, Kaunas University of Technology, Lithuania

Thermally activated delayed fluorescence (TADF) takes place in fluorescent molecules where the energy splitting between the lowest excited singlet and triplet state (ST-splitting, Δ_{ST}) is about $k_{\mathrm{B}}T$ at room temperature. Due to the small ST-splitting, the excited triplet states are easily converted into fluorescent singlet states via reverse intersystem crossing (RISC). This excitonic scheme is favorable for OLEDs, because it allows for making use of the large fraction of non-radiative triplets, which are formed under electroluminescence operation.
In this study, a new series of carbazol-donor-benzofluoride-acceptor complexes ("xFyCz") is introduced where x denotes the number of fluorine atoms saturating the acceptor and y is the number of carbozol donor groups. Various investigations are shown such as absorbance and photoluminescence spectroscopy in solution and thin films, solvatochromism as well as the application and performance study of the emitters in actual OLEDs including e.g. j-V and luminance measurements, power efficiency and external quantum efficiency (EQE) up to 12 % for 1F4Cz.

CPP 30.32 Tue 18:15 Poster B2

The effect of the fullerene LUMO position on the CT properties in polymer:fullerene blends — •Tobias Thiede, Jona Kurpiers, and Dieter Neher — Institute of Physics and Astronomy, Soft Matter Physics, University of Potsdam, Germany

In bulk heterojunction organic solar cells, one of the key parameters in solar cell efficiency, the open circuit voltage, has been shown to depend on the properties of the charge transfer (CT) state. These properties are again related to the energy gap between the highest occupied molecular orbital (HOMO) of the polymer and the lowest unoccupied molecular orbital (LUMO) of the fullerene acceptor. We present sensitive electroluminescence (EL) and external quantum efficiency (EQE) experiments on binary blends made of fluorinated copolymer 1F-PCPDTBT combined with the fullerene of different LUMO energy. By moving the LUMO of the fullerene we observe distinct changes in the absorption and emission properties. In particular, a significant increase of the EL efficiency accompanied by the appearance of emission from singlet excitons is seen when increasing the LUMO energy, as in blends with ICBA and ICTA. At the same time, the Voc loss due to non-radiative recombination is largely reduced. These findings help to understand the fundamental role of the energy landscape at the donor:acceptor interface and have important implications for designing future materials systems.

CPP 30.33 Tue 18:15 Poster B2

Ion sensing with electrochemical gated organic field effect

transistors based on diketopyrrolopyrrole polymers — •Benno Buchinger, Sven Hüttner, Anna Gräser, and Fabian Hoffmann — Universität Bayreuth, Organic and Hybrid Electronics, MC I

Since conjugated polymers have the potential for biosensor applications we investigated the possibility of building electrochemical and bottom gated organic field effect transistors for sensing applications using different conjugated polymers based on DPP (Diketopyrrolopyrrole) derivatives as active material. DPP polymers are a promising type of polymers as they allow a high tenability between high electron and hole transport with high charge carrier mobilities as well as a high stability in ambient and aqueous environments. Ions can either interact with the surface of the polymer layer or diffuse into the bulk and interact with functional corresponding hydrophilic groups, inducing changes in the electronic properties. This work addresses the feasibility to use these polymers for sensing applications, i.e. detect different ions and ion concentrations in aqueous environments important for a row of bio-sensing applications.

CPP 30.34 Tue 18:15 Poster B2

Low temperature charge transport characterisation of low band-gap diketopyrrolopyrrole (DPP) based polymers — •Fabian Hoffmann, Benno Buchinger, and Sven Hüttner — Universität Bayreuth, Organic and Hybrid Electronics, MC I

One of the most promising conjugated materials that emerged recently are conjugated polymers based on diketopyrrolopyrroles (DPP). Their semiconducting properties are directly related to their molecular ordering, molecular weight, purity and growth rate. In this context the material shows extraordinary high charge carrier mobilities in an OFET configuration due to the remarkable aggregating properties of the DPP moieties. Furthermore, they are stable at ambient conditions and can reach very low band gaps, which enables an absorption further in the red. At the same time they also show surprisingly low charge carrier mobilities in the bulk. We present temperature dependent OFET measurements to investigate the underlying charge transport processes. In particular, we address the influence of different processing conditions such as temperature and solvent vapour annealing.

CPP 30.35 Tue 18:15 Poster B2

Impact of PC[60]BM on the Photo-Degradation of PCPDTBT — Ulf Dettinger[1], Hans Joachim Egelhaaf[2], •Andreas Früh[1], Heiko Peisert[1], and Thomas Chassé[1] — [1]Eberhard-Karls-University, Institute for Physical and Theoretical Chemistry, Auf der Morgenstelle 18, D-72076 Tübingen, Germany — [2]ZAE Bayern, Haberstrasse 2a, 91058 Erlangen, Germany

Organic photovoltaics (OPV) offers a promising solution for the energy demand in combination with challenging design requirements, although the stability of the device materials remains yet an important factor. UV-Vis and FTIR spectroscopy was used to study the photooxidation of the Low-Band-Gap Polymer PCPDTBT as pristine film and blended with PC[60]BM. The films were degraded under irradiation of standard Air Mass 1.5 conditions under O2 environment. It has been shown that the different monomer units of the polymer backbone are differently affected by the degradation. The unique kinetics of the accelerated degradation of PCPDTBT in the blend is studied in detail.[1] Reference: [1]*U. Dettinger et al. Chem. Mater. 2015, 27, S. 2299-2308

CPP 30.36 Tue 18:15 Poster B2

Modeling the Exciton Diffusion in Flat Heterojunction Organic Solar Cells — •Karl-Philipp Strunk[1,2], Thomas Pfadler[1], and Lukas Schmidt-Mende[1] — [1]Universität Konstanz, Konstanz, Germany — [2]Centre of Advanced Materials, Heidelberg, Germany

Organic solar cells have proven themselves to be a promising candidate towards a more energy efficient future. The performance of flat heterojunction solar cells is limited by the exciton diffusion length L_D of the active materials. For this reason exact knowledge of L_D is of significant importance when comparing different organic semiconductors. In this work, an organic system with state-of-the-art performance employing an exciton blocking layer of Tris[4-(5-phenylthiophen-2-yl)phenyl]amine (TPTPA) is studied. Based on experimental and simulated external quantum efficiency (EQE) spectra, it is shown that TPTPA contributes to the photocurrent, although exciton blockers are commonly believed to be non-photoactive. EQE spectra are simulated using a transfer matrix approach and a generalized diffusion equation for the exciton density, following previous publications. Furthermore, simulated EQE spectra are fitted to experimental data to obtain values of L_D for both donor and acceptor. L_D of the donor is measured experimentally using a time-resolved photoluminescence technique. The good agreement of experimentally and computationally obtained exciton diffusion lengths proves the selected algorithm to be a unique way to determine L_D from measurements of complete devices along with material characterization and simulations.

CPP 30.37 Tue 18:15 Poster B2

Studying the Effects of Degradation in Organic Solar Cell Materials — •Michael Adams[1], Ian Howard[1], Bryce Richards[1], Andreas Weu[2], and Yana Vaynzof[2] — [1]Institute of Microstructure Technology, Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany — [2]Center for Advanced Materials, University Heidelberg, 69117 Heidelberg, Germany

Many factors have been reported to affect the stability of OPVs, among them are exposure to light, humidity, temperature and oxygen concentration. In order to develop strategies against these degrading effects we need to have a better understanding of the fundamental processes in the device's active layer. One of the most efficient OPV material combination to date is P3HT:PCBM. We perform transient absorption and streak camera measurements on P3HT:PCBM samples that have been prepared and degraded at the University of Heidelberg under various environmental conditions with the goal to identify differences in the photophysical processes occurring in these devices.

CPP 31: Hybrid and Perovskite Photovoltaics III (joint session CPP/DF/DS/HL, organized by DS)

Time: Wednesday 9:30–11:45 Location: H11

CPP 31.1 Wed 9:30 H11

Impact of Preparation Conditions on the Ionization Energy and Electronic Structure of CH3NH3PbI3 Perovskites — •Jennifer Emara[1], Tobias Schnier[1], Neda Pourdavoud[2], Thomas Riedl[2], Klaus Meerholz[1], and Selina Olthof[1] — [1]University of Cologne, Institute for Physical Chemistry, Luxemburger Straße 116, 50939 Köln, Germany — [2]Institute of Electronic Devices, University of Wuppertal, Rainer-Grunter-Straße 21, 42119 Wuppertal, Germany

Hybrid organic/inorganic halide perovskites have lately been a topic of great interest in the field of solar cell applications, with the potential to achieve device efficiencies exceeding other thin film device technologies. Yet, large variations in device efficiency and basic physical properties are reported. This is due to unintentional variations during film processing, which have not been systematically investigated so far. We therefore conducted an extensive study of the electronic structure of a large number of CH3NH3PbI3 perovskite films produced by different preparation methods and by varying precursor ratios. We show that variations in film stoichiometry lead to vast changes in the density of states (DOS), and changes in ionization energy, which can be intentionally tuned by almost 1 eV. Using x-ray diffraction measurements, we find the variations in film stoichiometry are not due to the formation of separate phases, but that interstitials and vacancies are homogeneously distributed within the material. Implementing the prepared perovskite layer materials in solar cells, we find a clear correlation between the changes in DOS with the overall power conversion efficiency.

CPP 31.2 Wed 9:45 H11

Two dimensional organometal halid perovskite nanosheets in light emitting application — •Rui Wang[1], Zhendong Fu[1], Vitaliy Pipich[1], Alexandros Koutsioumpas[1], Stefan Mattauch[1], Peter Müller-Buschbaum[2], and Henrich Frielinghaus[1] — [1]Jülich Center for Neutron Science, outstation at FRM II, Lichtenbergstr. 1, 85747 Garching — [2]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Two dimensional functional materials have created intensive research interest for high efficiency solar cells. Recently low dimensional perovskite nanocrystals, such as 2D perovskite nanosheets have been reported to possess reduced fluorescence decay times, an increased exciton binding energy and low conductivity in certain crystallographic directions. Consequently, these lower dimensional perovskites can be utilized for light emitting applications. In the present work, 2D nanosheet perovskites are formed by using octylamine bromide as capping ligands. GISANS combined with neutron reflectivity (NR) are applied to investigate the structure buried inside the thin films. GISANS had proven to be a powerful technique for thin film morphology investigations. NR guarantees that information about nanometer sized layers can be accessed. We present the determined structures in terms of optical properties, grain size information and stacked layered characteristic.

CPP 31.3 Wed 10:00 H11

Morphology and crystal orientation of hybrid perovskite thin films for application in high efficiency solar cells — •Johannes Schlipf[1], Lukas Oesinghaus[1], Nadja Giesbrecht[2], Yinghong Hu[2], Sigrid Bernstorff[3], Thomas Bein[2], Pablo Docampo[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Department of Chemistry and CENS, LMU München, 80539 München, Germany — [3]Elettra-Sincrotrone Trieste S.C.p.A., Basovizza, 34149 Trieste, Italy

Organo-metal halide perovskites mark a paradigm shift in photovoltaic research, as they combine high efficiencies challenging conventional inorganic solar cells with easy processing and cheap abundant precursor materials. Recent reports of power conversion efficiencies around 20% are possible due to remarkable material properties and their highly crystalline nature even when processed from solution. However, photovoltaic performance is directly linked to film morphology which in turn depends on the fabrication method. We investigate hybrid perovskite thin films of high efficiency solar cells prepared by various synthesis protocols with X-ray diffraction, GIWAXS and GISAXS. Thereby, we evidence different crystallization mechanisms that lead to certain morphologies and crystal orientations reflecting the chosen synthesis method [1]. We link these findings to the photovoltaic performance and aim at a rational development of new synthesis methods for high efficiency perovskite solar cells.

[1] Schlipf et al: J. Phys. Chem. Lett, 6, 1265-1269, 2015.

CPP 31.4 Wed 10:15 H11

Influence of annealing time on crystal structure and composition of CH3NH3PbI3-xClx mixed halide perovskite film — •Maryline Ralaiarisoa[1], Yan Busby[2], Johannes Frisch[1], Ingo Salzmann[1], Jean-Jacques Pireaux[2], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Brook-Taylor-Str. 6, 12489 Berlin, Germany — [2]Research Center in the Physics of Matter and Radiation , Laboratoire Interdisciplinaire de Spectroscopie Electronique (LISE), University of Namur, 5000 Namur, Belgium

Thermal annealing is a crucial step for the formation of crystalline perovskite films from precursor solution. However, the structural evolution during perovskite film formation and particularly its composition during annealing have not been thoroughly characterized yet. Such characterization is essential to understand the mechanisms leading to the complete conversion to perovskite. Using ToF-SIMS, we monitored the changes in composition and structure of CH3NH3PbI3-x Clx perovskite films after two different annealing stages, that is, before and after complete perovskite crystallization. At the early stage of annealing, our results show phase separation throughout the entire film depth into one where perovskite was formed and another where mostly the inorganic precursor PbCl2 was detected. After sufficiently long annealing, we found a single perovskite phase of homogeneous composition on the micrometer scale. By means of UPS, we further observed that perovskite films become more n-type for longer annealing time, which correlates the morphological evolution and the surface electronic structure.

15 min. break.

CPP 31.5 Wed 10:45 H11

Ferroelasticity in methylammonium lead halide perovskite? — Ilka Hermes[1], Simon Bretschneider[1], Victor Bergmann[1], Dan Li[1], Alexander Klasen[1,2], Julian Mars[1], Wolfgang Tremel[2], Frédéric Laquai[1], Hans-Jürgen Butt[1], Markus Mezger[1,2], Rüdiger Berger[1], Brian Rodriguez[3], and •Stefan Weber[1,2] — [1]MPI for Polymer Research, Mainz — [2]Johannes Gutenberg University, Mainz — [3]University College Dublin, Ireland

Methylammonium lead halide (MAPbX$_3$) perovskite materials show an outstanding performance in photovoltaic devices. However, some material properties, especially the possible ferroic behavior, remain unclear. We observed distinct nanoscale periodic domains in the piezoresponse of MAPbI$_3$(Cl) grains. The structure and the orientation of these striped domains is indicating ferroelasticity as their origin. By correlating vertical and lateral piezoresponse force microscopy experiments performed at different sample orientations with x-ray diffraction, the preferred domain orientation was assigned to the $a_1 - a_2$-phase. The observation of the twin domains appears to strongly depend on the preparation route and the film texture and is thought be induced by internal strain during the cubic-tetragonal phase transition.

CPP 31.6 Wed 11:00 H11

XPS study of the ALD growth of Al$_2$O$_3$ on the CH$_3$NH$_3$PbI$_3$ — •Małgorzata Sowińska[1], Chittaranjan Das[1], Konrad Wojciechowski[2], Henry Snaith[2], and Dieter Schmeisser[1] — [1]Brandenburgische Technische Universität Cottbus-Senftenberg, Angewandte Physik-Sensorik, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany — [2]Clarendon Laboratory, University of Oxford, Parks Road, Oxford, OX13PU, UK

Organic-inorganic lead halide perovskites have emerged as very attractive absorber materials for the fabrication of low cost and high efficiency solar cells, but a delicate nature of these films is one of the main challenges for a successful commercialization. Typically, when exposed to air or moisture, perovskite films degrade within a couple of hours or days. Moreover, the methylammonium lead triiodide (CH$_3$NH$_3$PbI$_3$) perovskite cannot sustain a prolonged annealing at temperatures around 85°C. In this work, we are investigating stability (upon air and thermal exposure) of a CH$_3$NH$_3$PbI$_3$ perovskite film coated with a thin layer of Al$_2$O$_3$ deposited by atomic layer deposition (ALD). In particular, the chemical and electronic changes occurred at the Al$_2$O$_3$/CH$_3$NH$_3$PbI$_3$ interface during the first 50 ALD cycles were monitored ex-situ by high-resolution and surface-sensitive synchrotron-based X-ray photoelectron spectroscopy (SR-XPS). The advantage of the ALD as a deposition method is that it can produce extremely dense layers with a very precise thickness control at room temperature. Detailed SR-XPS data analysis and a stability test of the perovskite film with alumina will be presented.

CPP 31.7 Wed 11:15 H11

Water based hybrid solar cells: spray deposition of the active layer monitored with x-ray scattering methods — •Volker Körstgens[1], Christoph Mayr[1], Stephan V. Roth[2], Hristo Iglev[3], Reinhard Kienberger[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]DESY Photon Science, Notkestr. 85, 22607 Hamburg — [3]TU München, Physik-Department, LS Laser- und Röntgenphysik, James-Franck-Str. 1, 85748 Garching

Spray-coating is a technique suitable for the large-scale and cost-effective preparation of hybrid photovoltaics. Unique environmentally friendly processing of hybrid solar cells can be realized with systems based on the solvent water. Using an active layer consisting of laser-ablated titania nanoparticles and water-soluble poly[3-(potassium-6-hexanoate)thiophene-2,5-diyl] (P3P6T) hybrid solar cells were realized. [1] For the performance of these devices the morphology of the active layer is of major importance. We followed the development of the morphology 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 of the active layer with increasing thickness and the dependence on the blocking layer chosen as the initial substrate are discussed and implications for an improved spray protocol will be given.

[1] Körstgens et al., Nanoscale 7, 2900 (2015).

CPP 31.8 Wed 11:30 H11

A low temperature route towards hierarchically structured titania films for thin hybrid solar cells — •Lin Song[1], Amr Abdelsamie[1], Christoph J. Schaffer[1], Volker Körstgens[1], Weijia Wang[1], Nicola Hüsing[2], Paolo Lugli[3],

and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Materialchemie, FB Chemie und Physik der Materialien, Universität Salzburg, Hellbrunnerstr. 34, 5020 Salzburg, Austria — [3]TU München, Department of Electrical Engineering and Information Technology, Institute for Nanoelectronics, 80333 München, Germany

Fabricating titania based solar cells at low temperature has a high significance regarding energy efficacy , since most of photovoltaic devices with titania require high-temperature calcination. Moreover, a low-temperature process offers the potential for flexible solar cells. However, this kind of solar cells has a low efficiency. In order to improve the device performance, we make superimposed structural order on titania films from nanometer to submicrometer length scales. Hierarchical structural order enhances light harvesting in solar cells, thereby enhancing the photovoltaic performance. Titania nanostructures are obtained via PS-b-PEO template assisted sol-gel processing. Nanoimprint lithography (NIL) provides ordered submicrometer patterns as a superstructure over nanostructured titania films. SEM and AFM measurements map the film surface morphology, and GISAXS measurements yield information about the bulk film morphology. The optoelectronic properties are examined by UV/Vis spectroscopy.

CPP 32: Focus: Triplet States in Organic Optoelectronics I

Organizers: Wolfgang Brütting (Universität Augsburg), Anna Köhler (Universität Bayreuth), Sebastian Reineke (Technische Universität Dresden)

The spin of Coulombically bound electron-hole pairs or excitons is of paramount importance for the functioning of organic optoelectronic devices. In particular, triplet states play an important role as radiative and non-radiative intermediates in organic light-emitting diodes and solar cells. This focus session addresses topical questions and recent progress in understanding the role of triplets in this field.

Time: Wednesday 9:30–12:45 Location: H37

Invited Talk CPP 32.1 Wed 9:30 H37

Towards 100% efficient OLEDs using thermally activated delayed fluorescence; how does the spin conversion work — •Andrew Monkman[1], Marc Etherington[1], Paul Klein[1,2], David Graves[1], Przemyslaw Data[1], Paloma dos Santos Lays[1], Roberto Nobuyasu[1], Youhei Tacked[3], and Fernando Dias[1] — [1]Durham University, Durham, England — [2]Technical University, Dresden, Germany — [3]Osaka University, Osaka, Japan

Detailed photophysical measurements of intramolecular charge transfer (ICT) states have been made both in solution and solid state. Temperature dependent time resolved emission, delayed emission and photoinduced absorption are used to map the energy levels involved in molecule decay, and through detailed kinetic modelling of the thermally activated processes observed, true electron exchange energies and other energy barriers of the systems determined with the real states involved in the reversed intersystem crossing mechanism elucidated.

For specific donor acceptor molecules, the CT singlet and local triplet states (of donor or acceptor) are found to be the lowest lying excited states of the molecule with very small energy barrier between them. In these cases the decay kinetics of the molecules become significantly different to normal molecules, and the effect of rapid recycling between CT singlet and local triplet states is observed which gives rise to the true triplet harvesting mechanism in TADF. Using a series of different TADF emitters we will show how the energy level ordering effects or does not effect TADF and how ultimate OLED performance is dictated by energy level ordering, from 5% to 22% EQE

CPP 32.2 Wed 10:00 H37

Thermally activated delayed fluorescence – A new route to more efficient OLEDs? — •Reinhard Scholz[1], Ramunas Lygaitis[1,2], Paul Kleine[1], Ludwig Popp[1], Florian Wüst[1], Simone Lenk[1], and Sebastian Reineke[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, Germany — [2]Department of Organic Technology, Kaunas University of Technology, Lithuania

In molecules with small splitting between the lowest excited singlet and triplet states, reverse intersystem crossing (RISC) from the triplet to the singlet requires only a small activation energy, resulting in thermally activated delayed fluorescence (TADF). Donor-acceptor compounds with large dihedral angle between these subgroups allow for rather low singlet-triplet splitting $\Delta_{\mathrm{ST}} = E(S_1 \to S_0) - E(T_1 \to S_0)$ between the observed fluorescence and phosphorescence transitions, at the price of a reduced transition dipole and slow radiative recombination rate. The present contribution investigates radiative recombination from thermal distributions in the excited potential surfaces S_n of TADF emitters with time-dependent density functional theory. On this basis, we suggest possible synthesis strategies for blue TADF emitters and report on selected compounds compromising between different desirable properties. The resulting OLEDs show external quantum efficiencies (EQE) between typical fluorescent and phosphorescent emitters, paving the way towards applications of white OLEDs to more efficient lighting.

CPP 32.3 Wed 10:15 H37

Biluminescence of purely organic semiconductors — •Caterin Salas Redondo, Simone Lenk, and Sebastian Reineke — Institut für Angewandte Photophysik, TU Dresden, Dresden, Germany

Biluminescence is a property of certain organic molecules, where light is emitted from both their singlet (named fluorescence) and triplet (named phosphorescence) excited states. Although the latter is a quantum mechanically forbidden transition, phosphorescence can be achieved if non-radiative channels are suppressed effectively. For instance, creating a simple host:guest system in which a biluminophore (i.e. materials with biluminescence property) is embedded in an optimum rigid matrix (e.g. polymers, small molecules), competitive thermal decay is suppressed, allowing emission from the triplet states in addition to the conventional fluorescence at room temperature. Not only the dual state emission is unique to this class of materials, but also the exciton dynamic range spanned by the two spin states is extreme, going from nanosecond-lifetime fluorescence up to second-lifetime phosphorescence.

In this presentation, we will report on our recent advances in different biluminescent systems. For example, we have identified a combination of PMMA[poly(methyl methacrylate)] as host and NPB[N,N di(naphtha-1-yl)-N,N diphenyl-benzidine] as biluminophore, giving rise to blue fluorescence and green phosphorescence. Additionally, we will report on the structure-property relationships between the host materials used and the resulting phosphorescence luminescence efficiency as well as the dependence of the persistent phosphorescence to oxygen.

CPP 32.4 Wed 10:30 H37

Understanding and predicting the orientation of heteroleptic phosphors in organic light-emitting diodes — •Tobias D. Schmidt[1], Matthew J. Jurow[2], Christian Mayr[1], Thomas Lampe[1], Peter I. Djurovich[2], Mark E. Thompson[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Department of Chemistry, University of Southern California, 90089 Los Angeles, USA

Horizontal orientation of dye molecules, i.e. their transition dipole vectors (TDV), is a powerful feature improving the efficiency of organic light-emitting diodes. In order to understand the underlying mechanisms for emitter orientation of heteroleptic phosphors, we compared the anisotropy factor of emissive guest/host systems using different Ir-complexes incorporating coumarin and phenylpyridin based ligands. These molecules exhibit similar high permanent dipole moments and electrostatic surface potentials but differ in the molecular structure. Interestingly, only molecules with aromatic and aliphatic ligands show non-isotropic distributions of their TDVs when co-deposited with a matrix material by thermal evaporation. From these findings we conclude that molecular orientation of heteroleptic Ir-complexes occurs instantaneously at the surface of the growing film and is driven by chemical interactions with the surrounding media. Furthermore, it was possible to predict the anisotropy factor for arbitrary molecular orientation with a mathematical model taking into account the geometrical distribution of the TDV on the molecules.[1]

[1] M. Jurow *et al.*, Nature Materials (2015), doi:10.1038/nmat4428

CPP 32.5 Wed 10:45 H37

Optical detection of spin states with dual singlet-triplet emitters in OLEDs — •Wolfram Ratzke[1], Lisa Schmitt[2], Philippe Klemm[1], Sebastian Bange[1], Sigurd Höger[2], and John Lupton[1] — [1]University Regensburg — [2]University Bonn

Doping OLEDs with dual emitters which exhibit simultaneous fluorescence and phosphorescence gives unique insight into spin statistics and dynamics. But bringing dipole forbidden triplets to light without perturbing the excited state of the organic semiconductor of interest and also conserving spin information requires a novel class of emitters. Typical phosphorescent molecules like heavy atom containing metalorganic complexes perturb their vicinity by the external heavy atom effect and destroy spin-coherence. Enhancing spin-orbit coupling by decreasing the singlet-triplet gap as exploited for TADF emitters is of limited utility for optical spin detection since singlet and triplet emission are hardly spectrally distinguishable and enhanced reversed intersystem crossing prevents spin-state preservation. Activating phosphorescence which is spectrally clearly shifted from singlet emission while preserving the spin state requires a more subtle principle. Here, we present metal-free dual emitters with well separated singlet and triplet emission. This separation enables the simultaneous investigation of singlet and triplet decay channels. The emitters can be used as sensing molecules giving a direct reading of the spin states. Changes in spin statistics by external manipulations, i.e. magnetic fields, can be optically detected.

15 min. break

Invited Talk CPP 32.6 Wed 11:15 H37

Effects of charge and exciton diffusion on triplet-polaron quenching and triplet-triplet annihilation in disordered organic semiconductors — •Reinder Coehoorn[1], Harm van Eersel[2], Le Zhang[1], Peter Bobbert[1], and Rene Janssen[1] — [1]Department of Applied Physics, Eindhoven University of Technology, P.O. Box 513 — [2]Simbeyond B.V., Den Dolech 2, 5612 AZ Eindhoven, The Netherlands

Triplet-polaron quenching (TPQ) and triplet-triplet annihilation (TTA) contribute to the efficiency roll-off in organic light-emitting diodes (OLEDs). In fluorescent OLEDs, TTA can also be beneficial, giving rise to partial triplet harvesting, which manifests itself as delayed fluorescence. Conventionally, TTA and TPQ are viewed as bimolecular processes with a rate coefficient which depends on the local density of all species involved, and on their diffusivity. Often, the rate coefficient is expressed in terms of an effective capture radius. We show from kinetic Monte Carlo simulations that in actual OLEDs strong deviations can occur from this picture. Firstly, the effective exciton or charge diffusion coefficient can be strongly time dependent. Secondly, the percolative nature of the charge or exciton diffusion gives rise to a highly non-trivial dye concentration dependence. For the case of TTA, results of an experimental study are presented which provide a test of a novel method [1] for quantifying the role of exciton diffusion. [1] H. van Eersel et al., J. Appl. Phys. 117, 115502 (2015).

CPP 32.7 Wed 11:45 H37

Electron-hole-pair magnetoresistance and magnetoelectroluminescence in OLEDs — •Hermann Kraus[1], Sebastian Bange[1], Ullrich Scherf[2], and John M. Lupton[1] — [1]Universität Regensburg, 93053 Regensburg, Germany — [2]Bergische Universität Wuppertal, 42119 Wuppertal, Germany

Large magnetoresistance 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. Spin resonance of paramagnetic species enables direct manipulation of charge carrier and excitonic precursor spins, providing a wealth of new insight into dynamic spin properties.

Previous work on electrical or optical detection of spin manipulation misses out on the opportunity to directly observe the presence of triplet exciton species that are at the heart of spin-dependent recombination models. Fortunately, a few organic materials are now known to exhibit reasonable triplet emission without modification of the polaron pair and exciton dynamics by strong spin-orbit interaction. They are ideal candidates to directly track spin singlet and triplet excitonic species in OLEDs under conditions of magnetic resonance, by comparing the fluorescence (singlet) to phosphorescence (triplet) intensity. Phosphorescence increases under resonance while fluorescence is quenched. Additionally, the magnetoelectroluminescence of the OLED can be measured at the same time by sweeping the magnetic field to directly correlate resonant and static magnetic field effects.

CPP 32.8 Wed 12:00 H37

Using deposition technique to control phosphorescent emitter orientation in doped organic films — •Thomas Lampe, Tobias D. Schmidt, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Introducing an overall horizontal orientation of transition dipole moments of heteroleptic Ir-complexes is a promising concept to improve efficiencies of organic light-emitting diodes. To investigate the impact of deposition technique on molecular orientation, we prepared doped films of four different phosphorescent iridium complexes in various organic host materials both by thermal evaporation and by solution processing and compared the observed emitter orientation. All heteroleptic Ir-complexes show comparable horizontal alignment if fabricated from the gas phase, while isotropic orientation or even a slightly vertical trend is observed in the solution processed samples. These findings can be explained by the creation of an interface between vacuum and the aromatic host material during evaporation and the lack of this feature when processed from solution. The underlying mechanism of molecular orientation can then be explained by the interaction of aliphatic and aromatic parts of the Ir-complexes with this interface during deposition from the gas phase. The absence of horizontal orientation of the phosphors in layers deposited from liquid preparation techniques has important implications for solution processed OLEDs.

CPP 32.9 Wed 12:15 H37

Active heterostructure of crystalline thin-film surface anchored metal-organic frameworks for optoelectronic applications — •Michael Oldenburg[1], Ian Arthur Howard[1,2], Andrey Turshatov[1], Nicolò Baroni[1], Stephanie Wollgarten[1], Engelbert Redel[3], Christof Wöll[3], and Bryce Sydney Richards[1,2] — [1]Institute of Microstructure Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]Light Technology Institute, Engesserstrasse 13, 76131 Karlsruhe, Germany — [3]Institute of Functional Interfaces, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Using surface anchored metal-organic framework (SURMOF) we could create a new kind of heterojunction. The process of triplet-triplet annihilation allowed us to track the triplets optically across the interface of the heterojunction. We are confident that this fundamental demonstration of selective transport over a SURMOF/SURMOF heterojunction will motivate further work in developing spray-on heterojunctions within the highly tunable SURMOF family that will have a wide variety of optoelectronic applications

CPP 32.10 Wed 12:30 H37

Recombination spectroscopy of organic solar cells by EDMR — Michael Eckardt[1,2], René Wieczorek[1,2], Frédéric Laquai[3], and •Wolfgang Harneit[1,2] — [1]Institut für Physikalische Chemie, JGU Mainz — [2]Fachbereich Physik, Universität Osnabrück — [3]KAUST, Saudi Arabia

Electrically Detected Magnetic Resonance (EDMR) is used to unravel different charge carrier recombination processes in P3HT:PCBM bulk heterojunction solar cells. Specifically, the dependence of the EDMR signal due to mobile P3HT polarons on electrical bias and illumination is correlated quantitatively to both, photo- and dark current of the cell. At moderate forward bias and all the way to reverse bias, solar cell operation and EDMR are dominated by recombination of photo-generated carriers. Near open circuit, injected charges accumulate near the electrodes, leading to additional recombination that depends strongly on details of fabrication and aging. EDMR allows quantifying this loss channel, which influences fill factor and maxiumum extractable power, with high precision.

CPP 33: Ionic Liquids and Water

Time: Wednesday 9:30–12:45 Location: H40

CPP 33.1 Wed 9:30 H40

Effect of Ionic Liquids on Aqueous Peptide Solutions: The Role of Anionic Interactions — •Diddo Diddens[1], Volker Lesch[2], Andreas Heuer[1], Christian Holm[3], and Jens Smiatek[3] — [1]Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster — [2]Helmholtz-Institut Münster: Ionics in Energy Storage Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster — [3]Institute for Computational Physics, University of Stuttgart, Allmandring 3, 70569 Stuttgart

We study the stability of a small β-hairpin peptide under the influence of an aqueous solution of various imidazolium-based ionic liquids (ILs). This is motivated by recent findings [1], which demonstrate that the IL 1-ethyl-3-methylimidazolium acetate (EMIM ACE) leads to denaturation of the native peptide structure. In particular, it was found that while the EMIM cation coordinates to both the folded and the unfolded peptide, the acetate anion predominantly interacts with the denatured state, thus shifting the folding-unfolding equilibrium. In this contribution, we therefore check the effect of different IL anions on the peptide structure by means of free energy calculations on the basis of MD simulation data. Our results are rationalized by the detailed coordination structure between the distinct co-solutes and the peptide.

[1] Lesch *et al.*, *Phys. Chem. Chem. Phys.*, **2015**, 17, 26049

CPP 33.2 Wed 9:45 H40

Structure of Ionic Liquids with $[\mathbf{C_nC_1im}]^+$ Cations — •Henning Weiss[1], Julian Mars[1,2], Hailong Li[1], Oxana Ivanova[3], Olaf Soltwedel[4], and Markus Mezger[1,2] — [1]Max-Planck-Institut für Polymerforschung, Mainz, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany — [3]JCNS at MLZ, Forschungszentrum Jülich, Garching, Germany — [4]Max-Planck-Institut für Festkörperforschung, Garching, Germany

The properties of ILs can be tailored by the selection of specific anions and cations. A common feature of ILs composed of cations with long aliphatic side chains are heterogeneities on the nanometer length scale. This so-called microphase separation arises from the clustering of aliphatic moieties. We used small angle neutron and x-ray scattering to study the liquid structure in a series of $[\mathrm{C_nC_1im}]^+$ based ILs with different anions. Analysis of the scattering pattern shows that the structural heterogeneities are governed by the interplay between the alkyl chain length and the geometry of the anion.

Invited Talk CPP 33.3 Wed 10:00 H40

Quasi-elastic neutron scattering study of an ionic liquid confined in nanoporous carbon — Mark Busch[1], Tommy Hofmann[2], Boris Dyatkin[3], Yuri Gogotsi[3], Alexei Kornyshev[4], Jan Embs[5], Bernhard Frick[6], and •Patrick Huber[1] — [1]TU Hamburg-Harburg, Hamburg, Deutschland — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Deutschland — [3]Drexel University, Philadelphia, U. S. A. — [4]Imperial College, London, UK — [5]Laboratory for Neutron Scattering, Paul Scherrer Institut, Villigen, Schweiz — [6]Institut Laue-Langevin, Grenoble, Frankreich

We present a quasi-elastic neutron backscattering study of the ionic liquid 1-N-butylpyridinium bis- ((trifluoromethyl)sulfonyl)imide [BuPy] [Tf$_2$N] confined in carbide-derived nanoporous carbon samples of different pore sizes. Elastic and inelastic fixed window scans while varying the temperature between 2 K and 350 K as well as quasi-elastic spectra acquired at selected temperatures allow us to infer the thermally-activated molecular mobility of the spatially nanoconfined ions.

CPP 33.4 Wed 10:30 H40

Polarization effects in molecular dynamics simulation of ionic liquids — •Volker Lesch[1,2], Andreas Heuer[2], Christian Schröder[3], Othmar Steinhauser[3], Hadrián Montes[4], Trinidad Méndez-Morales[4], Luis J. Gallego[4], and Luis M. Varela[4] — [1]Helmholtz-Institut Münster: Ionics in Energy Storage, FZ Jülich — [2]WWU Münster, Institut für physikalische Chemie — [3]University of Vienna, Department of Computational Biological Chemistry — [4]University of Santiago de Compostela, Departamento de Fisica da Materia Condensada

We report a molecular dynamics study of the effect of electronic polarization on the structure and single-particle dynamics of mixtures of the ionic liquid 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide doped with LiTFSI at room temperature. Therefore, we compare the predictions of the polarizable APPLE& P force field[1] with those of the standard non-polarizable OPLS-AA[2]. The structure of the mixtures is only weakly modified by the fluctuations in electron charge of their constituents, but their transport properties are indeed significantly changed. Moreover, the vibrational densities of states of the added cations are perturbatively red-shifted. A general theoretical framework for the calculation of polarization effects on the vibrational densities of states and velocity autocorrelation functions is introduced, which is useful for predicting the effect of the fluctuations of the electronic clouds on the transport coefficients of the system.

[1] O. Borodin, J. Phys. Chem. B, 113, 11463 (2009).

[2] W. L. Jorgensen, J. Phys. Chem., 90, 1276 (1986).

CPP 33.5 Wed 10:45 H40

Charge tranport and molecular dynamics in Polymeric Ionic Liquids — •Falk Frenzel[1], Makafui Folikumah[2], Matthias Schulz[2], Markus Anton[1], Wolfgang Binder[2], and Friedrich Kremer[1] — [1]Universität Leipzig, Leipzig, Deutschland — [2]Martin-Luther Universität Halle-Wittenberg, Halle (Saale), Deutschland

Polymeric Ionic Liquids (PIL) are synthesised by incorporating into telechelic Polyisobutylene (PIB)-based Ionic Liquid (IL)-like monovalent and bivalent cations of either N,N,N-triethylammonium or 1-methylpyrrolidinium with Br, NTf2, OTf and pTOS as anions. In total a homologous series of 16 PILs is studied. Charge transport, molecular dynamics and the microscopic structural arrangement are analyzed over a wide frequency (1E-2 - 1E7Hz)and temperature (200 - 400K) range by means of Broadband Dielectric Spectroscopy (BDS), Transmission Electron Microscopy (TEM) and Differential Scanning Calorimetry (DSC). Three relaxtion processes are observed: (i) the dynamic glass transition of the polymeric matrix, (ii) a conductivity relaxation originating from charge transport within IL-like moieties and (iii) a Debye-process tentatively caused by H-bonding-assembly; and in addition a weak electrode polarisation. The net conductivity of the PIL as a whole is quantitatively described by an Effective-Medium approach reflecting the microphase-separated character of the PIL under study.

15 min. break

CPP 33.6 Wed 11:15 H40

Impact of water on the charge transport of a glass-forming ionic liquid — •Pit Sippel, Victoria Dietrich, Daniel Reuter, Peter Lunkenheimer, Alois Loidl, and Stephan Krohns — Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany

Ionic liquids are salts showing melting temperatures below 100°C. These materials exhibit a variety of technically important physical and chemical properties, like electrochemical stability, low volatility, flame retardancy and ionic conductivity. Together with the immense number of ion combinations available for those ionic liquids, this makes them viable candidates for numerous applications, e.g., as electrolytes in energy applications, where their intrinsic ionic conductivity is an important feature [1]. However, water (and thus also ambient humidity) play a crucial role for the physical properties of ionic liquids, especially for the conductivity when hydrophilic anions are involved [2]. Using broadband dielectric spectroscopy and differential scanning calorimetry, we have investigated in detail the impact of small water volume-fractions on the conductivity and dynamical glass-properties of 1-Butyl-3-methyl-imidazolium chloride. We demonstrate that, by only slightly increasing the water content, glass transition temperature and conductivity are strongly enhanced and the dipolar dynamics are accelerated.

[1] D. R. MacFarlane, *et al.*, Energy Environ. Sci. **7,** 232-250 (2014).

[2] J. G. Huddleston, *et al.*, Green Chem. **3,** 156-164 (2001).

CPP 33.7 Wed 11:30 H40

Free interfaces in fluids of Ionic Liquid Crystals — •Hendrik

Bartsch[1,2], Markus Bier[1,2], and Siegfried Dietrich[1,2] — [1]Max Planck Institute for Intelligent Systems, Stuttgart, Germany — [2]University of Stuttgart, Germany

Recently, Ionic Liquid Crystals (ILCs) were attracting increasing scientific, as well as technological attention, since they are expected to exhibit unique structural properties, which are directly linked to the interplay of the anisotropy of the molecules, on the one hand, and their charges, on the other hand. Especially in inhomogeneous systems, e.g. fluids close to electrodes or free interfaces between fluid phases, this combination of properties can lead to new structures, which are not observable in ionic liquids or liquid crystals, separately.

Nevertheless, the theoretical understanding of the formation of interfaces in systems of ILCs is still incomplete. In particular, reliable predictions for the density and the nematic order parameter profiles are still rare. In order to address this open question, we study ILCs close to interfaces, by means of density functional theory. First, it will be shown that our approach resembles previous results for the bulk phase diagrams of charged and uncharged liquid crystals [1]. Ultimately, we will present new results on the free interface structure, for the liquid-gas and the smectic-liquid coexistence.

[1] S. Kondrat, M. Bier, and L. Harnau, J. Chem. Phys. **132**, 184901 (2010)

CPP 33.8 Wed 11:45 H40

Markov State Modeling for Water Dynamics — •Robert Schulz and Roland R. Netz — Freie Universität Berlin, Theoretical Bio- and Soft Matter Physics, Berlin, Deutschland

The unique properties of liquid water are relevant for a broad range of processes throughout many disciplines, e.g. protein folding. A long standing goal has been to relate the macroscopic properties such as the notable anomalies and singularities or transport properties to the microscopic structure, and thus to the hydrogen bonding pattern between individual molecules. We consider a Molecular Dynamics simulation of SPC/E water based on a 10ns long trajectory in bulk water. Pairs of water within a certain separation length R are considered and analyzed. With a Markov state model, we are able to discern different processes which describe switching of hydrogen bonds between different partners of water molecules. The application of transition path theory for discrete Markov chains reveal competitive reaction pathways when a hydrogen bond is broken and a new one is formed with another water molecule.

CPP 33.9 Wed 12:00 H40

Diffusion of charged species through water in confined environments: electronic structure and nuclear quantum effects — •Mariana Rossi[1,2], Michele Ceriotti[2], and David Manolopoulos[1] — [1]University of Oxford, Oxford, UK — [2]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

The diffusion and transport of protons and hydroxide ions through confined wires of water molecules are important processes both in biology (e.g. ion channels for pH regulation) and for technological applications (e.g. fuel cells). However, an atomistic theoretical understanding of the diffusion process from first principles – including the quantum nature of the nuclei – and the influence of the potential energy surface used to model it is still lacking. We treat here proton and hydroxide ions in isolated water wires of different lengths constrained by apolar cylindrical potentials with density functional theory potential energy surfaces. We use machine learning techniques [1] to identify the (often elusive) charged species and calculate diffusion coefficients including nuclear quantum effects, through path integral molecular dynamics techniques [2]. We propose a model to eliminate finite size effects and estimate the diffusion coefficients, finding that nuclear quantum effects play a role depending on the water-water separation in the potential energy surface, and is more accentuated for the hydroxide ions. [1] Gasparotto, Ceriotti, JCP **141**, 174110 (2014) [2] Rossi, Ceriotti, Manolopoulos, JCP **140**, 234116 (2014)

CPP 33.10 Wed 12:15 H40

The dielectric response of aqueous water slabs in nanoconfinement — •Alexander Schlaich, Philip Loche, Senta Volkenandt, and Roland R. Netz — Fachbereich Physik, Freie Universiät Berlin, 14195 Berlin, Germany

The dielectric constant of water in nanoconfinement is crucial for the emerging field of nanofluidics and nanochemistry, but also for modeling the electrostatic interaction between extended surfaces such as biological membranes. Furthermore the dielectric permittivity governs transport processes in protein crystals, nanotubes or clays.

The dielectric response at interfaces shows rich features that have profound influence on zeta potentials and capacitance. Using atomistic simulations at prescribed water chemical potential, we present spatially resolved dielectric profiles of water confined between hydrophilic surfaces and show that the water orientation becomes correlated in planar confinement, resulting in a drastic change of the local dielectric response tensor.

Simple modeling confirms that water orientation at the surface influences the response to an external field. The anisotropic dielectric response tensor leads to a modified prefactor of the Coulomb interaction for water in sub-nanometer confinement.

CPP 33.11 Wed 12:30 H40

Analysis of the Electronic Structure of Aqueous Urea and its Derivatives: A combined Soft X-Ray - TD-DFT Approach — •Marc F. Tesch[1], Ronny Golnak[1,2], Felix Ehrhard[1], Daniela Schön[1,2], Jie Xiao[1], Annika Bande[1], and Emad F. Aziz[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Freie Universität Berlin, Germany

For a comprehensive understanding of biophysical and chemical processes a detailed knowledge about a molecules electronic structure is essential. A powerful method to achieve this is the use of synchrotron radiation, which allows to investigate a sample on an element selective level. Here soft X-ray spectroscopic measurements combined with time dependent density functional theory calculations are presented to investigate the electronic structure of urea and its derivatives acetamide, thiourea, dimethylurea, and biuret. The molecules were dissolved in water to include solvent effects on the molecular structure. The focus of this study lies on X-ray absorption, emission, and resonant inelastic scattering measurements at the nitrogen K-edge. By combining these techniques information about the occupied and unoccupied molecular states can be obtained. It will be shown that for a proper interpretation of the experimental spectra it is crucial to consider the localized nature of the X-ray interaction at the nitrogen sites of the molecules and a thorough comparison to calculated spectra is inevitable. This is demonstrated by discussing the chemical relevant HOMO-LUMO gap, a property which is directly accessible from the measurements.

CPP 34: Crystallization, Nucleation, Self Assembly I (joint session CPP/DY, organized by CPP)

Time: Wednesday 9:30–12:15 Location: H42

Invited Talk CPP 34.1 Wed 9:30 H42

Polymer crystallization and nucleation: New insights from fast scanning calorimetry — •Christoph Schick[1], Evgeny Zhuravlev[1], and René Androsch[2] — [1]University of Rostock, Institute of Physics, 18051 Rostock — [2]Martin-Luther-University Halle-Wittenberg, Center of Engineering Sciences, 06099 Halle/Saale

Crystallization commonly starts from a (sub)nanoscale nuclei which eventually growth to a crystal. Classical nucleation theory (CNT) provides a qualitative description of these processes. Nevertheless, CNT often fails to predict nucleation and crystallization on a quantitative level. Differential scanning calorimetry (DSC) is often employed to probe such complex phase transitions. The traditional DSC is limited in its cooling capability to cooling rates below 10 K/s. However, many materials are crystallizing, e.g. during processing, at much faster cooling rates (100 to a few 1000 K/s). Knowledge about the phase transitions on fast cooling is therefore required. Chip based calorimeters cover this range but so far they do not allow to obtain the full information for fast crystallizing materials like PE or PTFE. Faster controlled cooling and heating rates above 106 K/s are therefore required. These novel fast scanning calorimeters were used in combination with conventional DSC to study crystallization of polymers on fast cooling, isothermal crystallization after fast quenches, the efficiency of nucleating agents, the kinetics of crystal nucleation and the kinetics of the glass transition. The basic principle of the new technique and applications to polymeric and non-polymeric materials will be presented.

CPP 34.2 Wed 10:00 H42

Elementary steps of chain folding in a melt of linear polyethylene * a proposal for discussion. — •Heinz H. W. Preuss — Sedanstr. 6, 31785 Hameln

As far as lamellae of crystalline polyethylene from solution or melt consist of close folded molecular chains (Preuss DPG Spring Meeting 2015, CPP 6.7), one has to find out how the folding can occur. The answer is in the understanding of the limited mobility and flexibility of polymer molecules in a melt. If the molecules are with a large portion nearly close and parallel packed, they can move freely in the direction of their backbone by *worming*(Faraday Discussion 1979, F. C. Frank, p 7 ff., A. Keller, p.146 ff.).In the direction perpendicular to the backbone, molecules have 8,5 % (1/12)of their diameter as average room of move for isomeric exchange of the place of C and H atomes. By simultaneous exchange of some C-H-pairs one can get pairs of folds in an extended chain keeping its general orientation. This would be possible with small molecules neighbouring only and should occur already during polymerization in solution or gas. The expression *adjacent reentry* is in this context a source of missunderstandig, for it provokes the meaning, molecules would move out of the place of junktion in a lamella and would reenter nearby after returning, a probably impossible motion.

CPP 34.3 Wed 10:15 H42

How realistic are *random coils* in HD-PE? Analysis of the closeness of the packing. — •Heinz H. W. Preuss — Hameln

In a previous talk (CPP 6.7 Spring Meeting 2015) was demonstrated evidence of chain folding in HD-PE after slow cooling from the melt. With an analysis of the density and closeness of Packing including a model experiment with balls close wound with a clothes line one can learn that the density of the melt can be reached only with a high portion (at 80 %) of chain segments beeing nearly close and parallel neigbouring but not with *random coils* understood as balls packed with an entangeled molecular chain. The conformation in the melt should be near to the conformation in the crystal what is easy to be understood with the existence of folded chains in the melt. Compared with the crystal structure in the melt the molecules have 27,6 % more volume and 8,5 % more average distance available for mobility and flexibility. The random coil remains an important abstract mathematical tool, but should not be missinterpreted as if an arbitrarily coiled line could be a correct model of polymer molecules in a melt.

CPP 34.4 Wed 10:30 H42

Wang-Landau simulation of short single polyethylene chain's "crystallization" — •Timur Shakirov and Wolfgang Paul — University of Halle, Halle, Germany

The phase behaviour of polyethylene has been under wide investigation during the last 6 decades. But investigation of single chain crystallization is a technically difficult problem. In the case of molecular dynamics simulations, it is not so easy to distinguish kinetic and thermodynamic effects on chain folding. We present results of a Wang-Landau type Monte Carlo study at thermodynamical equilibrium of folding of a single polymer chain. Our simulations are based on a chemically realistic united atom model [1].

[1] W. Paul, D.Y. Yoon, G.D. Smith. An optimized united atom model for simulations of polymethylene melts. The Journal of chemical physics, 103(4), 1702-1709. (1995)

15 min. break

CPP 34.5 Wed 11:00 H42

Control of homogeneous crystal nucleation in polymers — •Evgeny Zhuravlev[1], Jürn Schmelzer[1], René Androsch[2], and Christoph Schick[1] — [1]University of Rostock, Institute of Pysics, Wismarsche Str, 43-45, 18057 Rostock — [2]Martin-Luther-University Halle-Wittenberg, Center for Engineering Sciences, 06099 Halle/S., Germany

A summary of recent application of Tammann's nuclei development method [1] to fast crystallizing polymers has been laid out to further address the role of pre-formed homogeneous nuclei on crystallization kinetics as well as semi-crystalline morphology. Making use of the separation in time of homogeneous nucleation and growth in the vicinity of glass transition temperature, the nuclei can be pre-formed using the precision and fast temperature control of a fast scanning calorimeter [2]. Further non-isothermal and isothermal heat treatments of these nuclei largely affects on crystallization kinetics and morphology. Combination of these studies contributes to a better understanding of homogeneous nuclei volume density, thermal stability and reordering kinetics. [1] Tammann, G., Number of nuclei in supercooled liquids. Zeitschrift für Physikalische Chemie 1898, 25, 441-479; [2] Zhuravlev, E., et al., Experimental test of Tammann's nuclei development approach in crystallization of macromolecules. Crystal Growth & Design, 2015. 15(2): p. 786-798.

CPP 34.6 Wed 11:15 H42

Crystallization behavior of nanocomposites based on Polylactide - Rigid Amorphous Phase due to the Nanofiller — •Jing Leng[1], De-Yi Wang[2], Andreas Wurm[3], Christoph Schick[3], and Andreas Schönhals[1] — [1]Bundesanstalt für Materialforschung und prüfung — [2]IMDEA Materials Institute — [3]University of Rostock, Institute of Physics

Two kinds of synthesized NiAl (NiAl-LDH) and MgAl (MgAl-LDH) layered double hydroxides were melt blended with commercial polylactide to prepare different polymer based nanocomposites. The MgAl-LDH based nanocomposites and NiAl-LDH based nanocomposites have a different but mixed intercalated / exfoliated structure. Based on the different structures, the crystallization behaviors of polymer based nanocomposites were investigated by differential scanning calorimetry (DSC) and temperature modulated differential scanning calorimetry (TMDSC) specificly where the heating and cooling rates were varied in a considerably wide range. In a first step, the cooling rate where crystallization can be completely surpressed is estimated. In a second step, based on a specified temperature program the crystalline fraction (CF), the rigid amorphous fraction (RAF) and the mobile amorphous fraction (MAF) were calculated from the the enthalpy and specific heat capacity in dependence on the concentration of the nanofiller. The rigid amorphous fraction was considered as resulting from the the crystallites and the nanofiller. For the first time both fractions were calculated quantitatively without any additional assumption.

CPP 34.7 Wed 11:30 H42

Improved Transferability of Coarse Grained Models for Polymer Crystallization Using Machine Learning — •Chan Liu[1], Christine Peter[2], Kurt Kremer[1], and Tristan Bereau[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Theoretical Chemistry, University of Konstanz, Konstanz, Germany

Coarse-grained (CG) models, which combine a number of atoms into superatoms or beads, can significantly speed up the simulations and provide reasonable resolution for studying polymer crystallization. One of the major challenges in CG modeling is that the reduction of the number of degrees of freedom makes the resulting coarse models state point dependent; that is, most CG force fields developed from the structures of an atomistic melt are not guaranteed to be transferred to crystalline structures. Thus deriving a transferable CG potential across different thermodynamic states is rather crucial if one want to study the phase behavior of polymeric systems. In this work, we introduce a Machine Learning approach to improve an existing CG model parametrized for a different phase by predicting the deviation between CG and atomistic forces, which can be seen as an external force added on the original CG force field. This model predicts a force on each bead based on the surrounding geometry without projecting it onto pairwise potentials such that it can potentially reproduce many-body contributions. This approach opens the perspective to modeling many-body interactions in CG simulations and thus improve the transferability and accuracy of its force field.

CPP 34.8 Wed 11:45 H42

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

Nanostructures of semi-crystalline diblock copolymers (DBCP) can be tailored by controlled crystal thickening. In double-crystalline DBCP, both blocks have the ability to crystallize and, thus, can be used for crystal thickening which was not investigated so far. The aim of the study was to test the hypothesis that the lamellar long period of a linear double crystalline polyethylene-block-poly(ethylene oxide) (PE-b-PEO) can be increased by stepwise annealing of both crystalline phases. Using differential scanning calorimetry, one-step annealing experiments revealed crystal thickening of both crystalline phases, PE and PEO, separately. X-ray scattering experiments showed that PEO crystal thickening did not affect the PE-b-PEOs morphology while PE crystal thickening increased the lamellar long period. Crystal thickening of both phases together was realized by two-step annealing which further increased the lamellar long period as compared to the sole PE crystal thickening. This observation was attributed to a stretching of PEO-blocks triggered by the initial PE crystal thickening that enabled the formation of thicker PEO crystals compared to the one-step annealing of PEO. The defined crystal thickening of double-crystalline DBCP can be used to fabricate tailorable nanopatterns for materials science applications in photonics or the biomedical field.

CPP 34.9 Wed 12:00 H42

Interface & confinement induced order and orientation in thin films of Poly-Caprolactone — •Wilhelm Kossack[1], Anne Seidlitz[2], Thomas Thurn-Albrecht[2], and Friedrich Kremer[1] — [1]Universität Leipzig, Institute for exp. physics 1,04103 Leipzig — [2]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, 06120 Halle/Saale

Infrared-transition moment orientational analysis (IR-TMOA), X-ray Diffraction (XRD) measurements and model calculations are combined to study interface and confinement induced order and orientation in thin ($h \approx 11 \times 10^{-6}$ m) films of Poly-caprolactone (PCL) prepared by drop-casting on silicon wafers. Depending on the crystallization temperature, 303 K $\leq T_x \leq$ 333 K, spherulites with a diameter of 1×10^{-6} m $\leq d_S \leq 500 \times 10^{-6}$ m form. Macroscopic order of the crystalline lamellae is imposed by spatial ($d_S > h$) and interfacial interactions and quantified IR-TMOA and XRD pole figures. Both techniques rely on the relative orientation of sample and incident radiation, and measure, in case of PCL, the orientation distribution of *complementary* crystal directions. This allows to (1) correlate the directions of the transition moments with the crystal axes; and (2) estimate the volume fractions of flat- or edge on lamellae as induced by the different interfaces, as well as the fractions of surface-induced- or bulk-nucleated spherulites in dependence on T_x. The contribution of substrate induced spherulitic structures rises with $T_x = 323$ K up to ~ 12 vol%, whereas no indications of edge on lamellae at the free surface are found. The bulk phase, on the other hand, dominates at $T_x \leq 313$ K.

CPP 35: Activated and Glassy Dynamics of Soft Matter (joint session CPP/DY, organized by CPP)

Time: Wednesday 9:30–13:00 Location: H51

CPP 35.1 Wed 9:30 H51

On the dynamics of densely grafted polymer chains — •Michael Lang, Marco Werner, Ron Dockhorn, and Torsten Kreer — Leibniz Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden, Germany.

Large scale Monte Carlo simulations of a dense layer of grafted polymer chains in good solvent conditions are used to explore the dynamics of a "polymer brush". Monomer displacements are analyzed resolving the directions parallel and perpendicular to the grafting plane. Autocorrelation functions of segment and partial chain end-to-end vectors are analyzed as function of time. We demonstrate that the terminal relaxation time τ of entangled chains with a degree of polymerization N in a brush is related to the entanglement degree of polymerization, N_e, via $\tau \propto N^3 \exp(N/N_e)$. The confining tube in the brush is similarly stretched as the chain conformations with tube diameters perpendicular and parallel to the grafting plane related by $a_\perp \approx a_\parallel (N_e/g)^{1/2}$, whereby g is the number of monomers per correlation volume of the brush. One specific effect of the confining potential is that the terminal part of the perpendicular component of the monomer position vector auto-correlation function decays simultaneously for all monomers.

CPP 35.2 Wed 9:45 H51

Transient Cooperative Process in Dewetting Polymer Melts — •Sivasurender Chandran and Günter Reiter — Institute of Physics, Albert–Ludwig University of Freiburg, Freiburg, Germany

Polymer melts exhibit a rich dynamic behavior when exposed to intense shear fields. For example, amorphous polymers display a shear thinning behavior, while crystallizable polymers form correlated segments within the flow induced oriented structures. However, the role of such correlations on the dynamic behavior of crystallizable polymer melts is highly unexplored.

To explore this crucial aspect, we have compared the high velocity dewetting (*shearing*) behavior of molten amorphous (atactic polystyrene, aPS) and crystallizable (isotactic polystyrene, iPS) polymer films, above the melting point. For aPS, the apparent viscosity of the films (η_f) derived from dewetting was less than zero shear bulk viscosity (η_{bulk}), displaying the expected shear thinning behavior. Surprisingly for iPS films, η_f was always larger than η_{bulk}, even at about 50 °C above the melting point, with $\eta_f/\eta_{\mathrm{bulk}}$ following an Arrhenius behavior. The corresponding activation energy of $\sim 160 \pm 10$ kJ/mol for iPS films suggests a cooperative motion of segments which were aligned and agglomerated by fast dewetting. These observations were not anticipated by standard models and hence indicate to the need for a new concept in polymer physics.

CPP 35.3 Wed 10:00 H51

Picosecond Dynamics of Liquid Glycerol Above T$_g$ — •Sebastian Busch[1], Alessandro Vispa[2], Nicolas Giovambattista[3], and Luis Carlos Pardo[2] — [1]German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Geesthacht GmbH, Lichtenbergstr. 1, 85747 Garching bei München, Germany — [2]Departament de Física i Enginyeria Nuclear, Universitat Politècnica de Catalunya, Barcelona, Spain — [3]Physics Department, Brooklyn College of The City University of New York, Brooklyn, USA

An understanding of the dynamics of glass-forming liquids at temperatures significantly above the glass transition still represents a much-coveted goal. If any theory or explanation is to be extrapolated to understand the undercooled regime from knowledge of high-temperature equilibrium states, a consensus must first exist on the underlying physics of the liquid phase at temperatures above the glass transition.

The aim of this work is to provide a detailed and critical appraisal of two specific questions about the dynamics of liquid glycerol, a prototypical glass-forming liquid: The first one concerns how many distinct dynamical processes are present in glycerol in the sub-nanosecond regime. The second one concerns whether a homogeneus (dynamically driven) or heterogeneous (structurally driven) scenario better describes Quasielastic Neutron Scattering data and Molecular Dynamics simulations.

A. Vispa et al., "A Robust Comparison of Dynamical Scenarios in a Glass-forming Liquid", PhysChemChemPhys, accepted.

CPP 35.4 Wed 10:15 H51

Mechanically induced ageing and compaction of porous polymer membranes — •Ulrich A. Handge — Helmholtz-Zentrum Geesthacht, Institut für Polymerforschung, Max-Planck-Strasse 1, 21502 Geesthacht

The permeability of porous polymer membranes often is reduced by mechanical compaction caused by the applied pressure. This process is strongly determined by the viscoelastic properties of the polymer and its plasticization caused by the feed medium. In this work, the time-dependent compaction of porous polymer membranes under pressure is modelled. We focus on the influence of viscoelastic and diffusion properties of the polymer material on compaction and on the decrease of membrane permeability with time. Different membrane morphologies are discussed. The life-time of a porous polymer membrane is associated with the time at which the glass transition is achieved in a creep experiment. We calculate the maximum life-time of polymer membranes based on compaction. The analysis of our model reveals that the diffusion coefficient, the average retardation time in creep, the magnitude of creep compliance and the time-temperature-pressure shift factor strongly influence the pressure induced compaction of microporous membranes. Generally, a larger tortuosity at constant porosity leads to a lower life-time of the membrane. Buckling of cell struts is the dominant failure mechanism in porous membranes with a very high porosity.

CPP 35.5 Wed 10:30 H51

Lifetime Prediction of Physical Ageing in Glassy Polymer Membranes — •Nils Müller[1], Ulrich Alexander Handge[1], and Volker Abetz[1,2] — [1]Helmholtz-Zentrum Geesthacht, Institute of Polymer Research, Geesthacht, Germany — [2]University of Hamburg, Institute of Physical Chemistry, Hamburg, Germany

The long-term performance stability of glassy polymer membranes is strongly affected by physical ageing. Therefore, we investigate the lifetime evolution of membrane properties through the application of the ageing model developed by Struik [1] and the statistical analysis thereof [2]. We propose several lifetime definitions suitable for membrane characterisation. The bootstrapping method is used in our analysis of the influence of a reduction of the data points used in model fitting on prediction quality. In this context we discuss the interdependency of experimental time expenditure and choice of model parameters with regard to lifetime prediction. A dimensional analysis of the Struik equation yields a master curve concerning the accelerated ageing behaviour of thin films. Our analysis of the master curve reveals a weak dependence of the membrane lifetime on initial conditioning. Dependent on the lifetime definition, we find a varying relationship between lifetime and relaxation time ranging from proportional to inverse proportional.

[1] L.C.E. Struik (1978). Physical aging in amorphous polymers and other materials.

[2] N. Müller, U.A. Handge, and V. Abetz (2015). Physical ageing and lifetime prediction of polymer membranes for gas separation processes. Submitted for publication.

15 min. break

Invited Talk CPP 35.6 Wed 11:00 H51

The extraordinary mechanical properties of spider silk and it's molecular foundation — •Friedrich Kremer[1], Markus Anton[1], Periklis Papadopoulos[2], Roxana Figuli[3], and Wilhelm Kossack[1] — [1]Universität Leipzig — [2]Max-Planck-Institut für Polymerforschung, Mainz — [3]Karlsruher Institut für Technologie (KIT), Karlsruhe

Spider silk is a high-performance fiber with unique mechanical properties which are currently not met by man-made materials. It consists essentially out of two proteins, major ampullate spidroin1 and spidroin2, having alanine-rich blocks interrupted by glycine-rich sequences. The former assembles to ß-sheeted nanocrystals which are embedded in the amorphous chains of the latter and which are interlinked by a ~ 10 % fraction of prestressed chains. This causes within the fiber a negative inner pressure which is counterbalanced by the matrix surrounding the fibrils and by the outer skin. Wetting of the fiber results in a spontaneous "supercontraction" into the equilibrated state. - In the talk a detailed description of this interplay between inner and outer constraints will be discussed based on a variety of complementary experimental methods like polarized, time-resolved FTIR-spectroscopy, measurements of the mechanical modulus and micro-X-ray scattering. It enables one to deduce a quantitative model describing the macroscopic response in the dependence on the microscopic parameters.

CPP 35.7 Wed 11:30 H51

Tayloring the properties of polydiene elastomers via associating hydrogen bonding groups: A micro- and macroscopic approach — •Barbara J. Gold, Claas H. Hövelmann, Wim Pyckhout-Hintzen, Andreas Wischnewski, and Dieter Richter — Forschungszentrum Jülich, JCNS-1 & ICS-1, 52425 Jülich, Germany

Nature uses a combination of dynamic hydrogen and static covalent bonds e.g. in the muscle protein TITIN [Wojtecki et al., Nature Materials 2011] to achieve toughness in otherwise elastic materials. We transferred this mechanism into conventional elastomers by introducing associating hydrogen bonds into covalent crosslinked polydiene networks. Since the associating behaviour of these functional groups can be triggered by temperature or mechanical stimulation this new generation of elastomers serves as key actor for the design of novel knowledge-based materials.

The influence of the hydrogen bonding groups on the dynamics of linear polymer chains has been studied by oscillatory shear rheology, dielectric and neutron spin echo spectroscopy. We observe a clear influence on the relaxation time spectra resulting in a longer disentanglement time, higher segmental friction as well as a second relaxation process related to the lifetime of the associating groups. Furthermore the Gaussian chain structure, observed via small angle neutron scattering, remains unaffected which excludes phase separation within the material. Stress-strain investigations show a significant increase of the mechanical resistance due to the additional functional groups compared to conventional elastomers.

CPP 35.8 Wed 11:45 H51

Chain-level dynamics and relaxation in supramolecular self-healing networks — Anton Mordvinkin and •Kay Saalwächter — Institut f. Physik-NMR, Martin-Luther-Univ. Halle-Wittenberg, Betty-Heimann-Str. 7, 06120 Halle, Germany

We elucidate the relationship between the local "sticker lifetime" and the mechanical properties of different polyisobutylene (PIB) based supramolecular elastomers with self-healing capability [1,2]. The systems comprise linear PIB end-functionalized with hydrogen-bonding units [1] and randomly functionalized with ionic side groups [2]. In both cases, the supramolecular groups form clusters that correspond to high-functionality crosslinks, rendering the relationship between local bonding-debonding dynamics and the rheological behavior complex. We study the chain-level dynamics using an NMR-based molecular rheology approach [3]. Our results provide the microscopic underpinning of the rheological properties, and show the first direct evidence of "sticky reptation" [4] in the randomly functionalized ionomer case.

[1] T. Yan et al., *Macromolecules* **47**, 2122 (2014)

[2] A. Das et al., *ACS Appl. Mater. Interf.* **7**, 20623 (2015)

[3] F. Vaca Chavez, K. Saalwachter, *PRL* **104**, 198305 (2010)

[4] M. Rubinstein, A.N. Semenov, *Macromolecules* **34**, 1058 (2001)

CPP 35.9 Wed 12:00 H51

A novel approach to determine the cross-linking level of epoxy resins — •Lisa Maria Uiberlacker, Moritz Strobel, and Sabine Hild — Johannes Kepler University Linz, Institute of Polymer Science, 4040 Linz, Austria

The cross-linking density of epoxy resins is a crucial parameter that determines its mechanical properties and characteristic data such as the glass transition temperature. Typically, the glass transition temperature increases with increasing cross-linking level of the epoxy system. A direct measurement of glass transition temperature is possible with DSC, but the cross-linking level has to be calculated from the remaining enthalpy compared to a completely cured sample. Raman spectroscopy is often used for the determination of the cross-linking density of epoxy resins. The decrease of the epoxide vibration peak is compared to the vibration peak of the phenyl ring peak, which is not affected by the curing of the epoxy system. Our approach is to determine the glass transition temperature of the resin with various crosslinking levels using an AFM equipped with a heatable cantilever. Performing local thermal analysis is based on a temperature calibration with known polymer standards to correlate the tip temperature with the applied voltage on the tip. AFM has a high spatial resolution which allows the determination of local differences in the glass transition temperature. The local thermal analysis with AFM is compared with conventional methods like Raman spectroscopy and DSC.

CPP 35.10 Wed 12:15 H51

Supramolecular association in transiently branched polymer systems — •Mariapaola Staropoli, Claas Hoevelmann, Juergen Allgaier, Andreas Raba, Wim Pyckhout-Hintzen, Andreas Wischnewski, and Dieter Richter — JCNS-1 Forschungzentrum Juelich

In this contribution, the investigation of hydrogen bonding mechanism in a transiently branched comb-like polymer system, is presented. The system under investigation consists of a polybutylene oxide (PBO) based backbone, randomly functionalized with thymine (Thy) groups, in combination with shorter PBO chains, end functionalized with Diaminotriazine (Dat) groups. The functional groups are able to associate through hydrogen bonds. The complementary association of these groups leads to the formation of a transiently branched comb-like polymer system. The interaction of hydrogen bonding groups in the melt state has been studied on microscopic level by Small Angle Neutron Scattering technique (SANS), by mean of the selective labeling scheme.A peak observed in the scattering function, reveals the formation of a block copolymer, due to the complementary association of the hydrogen bonding groups. The scattering profile of a block copolymer is described by mean of RPA formalism through which it is possible to obtain an average aggregation number in the melt and thus, the association constant. Rheological measurements in the melt have been performed in order to study the influence of the transient bonds on the macroscopic properties of the polymer system and to analyze the effect of the reversible interaction on the dynamic.

CPP 35.11 Wed 12:30 H51

ReaxFF+ I - a new reactive force field method for the accurate description of ionic systems — •Oliver Böhm[1], Stephan Pfadenhauer[1], Roman Leitsmann[1], Philipp Plänitz[1], and Michael Schreiber[2] — [1]AQcomputare GmbH, Annabergerstr. 240, 09125 Chemnitz — [2]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

We present a powerful extension of the reactive force field method ReaxFF which we call ReaxFF+ . We have implemented a new charge equilibrium scheme which takes into account different bond types yielding different screening factors. The main advantage of this procedure is the correct distinction and description of covalent and ionic bonds. Therefore, it is the only force field that allows reactive molecular dynamic simulations in ionic gases and liquids.

CPP 35.12 Wed 12:45 H51

ReaxFF+ II - highly efficient parametrization methods for the ReaxFF+ at the example of the hydrolysation of aluminosilicates — Oliver Böhm[1], Stephan Pfadenhauer[1], •Roman Leitsmann[1], Philipp Plänitz[1], and Michael Schreiber[2] — [1]AQcomputare GmbH, Annabergerstr. 240, 09125 Chemnitz — [2]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

One of the biggest challenges for using force fields is to find a suitable parametrization according to the chemical or physical problem. Especially in the ReaxFF+ method several hundred parameters have to be fitted. Therefore, the development of efficient optimization methods is the key for a successful application of reactive force fields in general and of the ReaxFF+ method in particular. We present a fast multidimensional optimization method which is parallelized using OpenMP. Moreover, we introduce an automatic training scheme which allows a continuous improvement of the training set as well as the identification of critical properties and non fittable properties. The method will be demonstrated by the example of the hydrolisation of aluminosilicates.

CPP 36: Complex Fluids and Colloids V (joint session BP/CPP/DY, organized by DY)

Time: Wednesday 10:00–13:00 Location: H47

CPP 36.1 Wed 10:00 H47

Self-assembly in binary mixtures of liquid-crystalline rods and dipolar spheres: A free-energy study — •Alice C. von der Heydt, Stavros D. Peroukidis, and Sabine H. L. Klapp — Inst. f. Theoretische Physik, Techn. Univ. Berlin, Hardenbergstr. 36, 10623 Berlin

Mixtures of differently shaped particles with hard-core repulsion only can exhibit a variety of spatially periodic phase-separation patterns combined with liquid-crystalline order [1]. Simulations have revealed an even more complex behavior with uni- or biaxial, smectic and lamellar structures in binary mixtures of rods and soft magnetic spheres of comparable diameter [2]. In this study, we aim at a theoretical description that will allow us to trace phase boundaries and to explain topologies of some of these structures for a model mixture of hard rods with nematic order and dipolar hard spheres. The semi-analytical route we propose starts from a free-energy functional which governs the single-particle component-density distribution functions of position and orientation. This functional is constructed using concepts of classical density functional theory and the modified mean-field approximation for the dipolar interaction [3].

[1] Z. Dogic, D. Frenkel, S. Fraden, Phys. Rev. E **62**, 3925 (2000)
[2] S. D. Peroukidis, K. Lichtner, S. H. L. Klapp, Soft Matter **11**, 5999 (2015)
[3] G. M. Range, S. H. L. Klapp, Phys. Rev. E **69**, 041201 (2004)

CPP 36.2 Wed 10:15 H47

Clogging in a microfluidic hourglass — •Alvaro Marin[1], Massimiliano Rossi[1], Henri Lhuissier[2], and Christian J. Kähler[1] — [1]Institut für Strömungsmechanik und Aerodynamik, Universität der Bundeswehr München — [2]IUSTI - Aix-Marseille Université & CNRS

Mass flows through geometric constrictions tend to clog under certain circumstances, it occurs no matter what type of object you consider: sand in an hourglass, particles in a fluid through a porous medium or people leaving a room (Zuriguel et al., Scientific reports 4, 2014). However, it is well-known that hourglasses work optimally when the particle-to-neck ratio is within certain ratio without interruption, while arching occurs for particle-to-neck ratios above. In the case of porous mediums, filters and membranes, these get easily clogged by particles in the fluid and therefore unfunctional after a certain amount of time. Being the only solution the replacement of the membrane/filter. Certainly the adherence of the particles to the walls and to each other is an important parameter, but even in the case without adherence, the clogging probability is far from negligible. To study these regimes, we study microfluidic devices with a bottleneck of squared cross-section through which we force dilute polystyrene particle solutions with diameters comparable to the bottleneck size and down to one tenth its size. The experimental results show that particles flowing through a geometrical constriction in these conditions (as it occurs with the flow in certain filters and membranes) reveals strong statistical similarities with an hourglass, which is explained with a simple statistical model.

CPP 36.3 Wed 10:30 H47

Viscoelastic properties of marginal networks in a solvent — •Matthew Dennison and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany

Elastic networks that are at the margins of mechanical stability are known to exhibit an anomalously large resistance to deformation which is highly sensitive to applied forces and fields. While many previous studies have examined the static properties of such networks, relatively little is known about their dynamical behavior. Using a hybrid molecular dynamics and multi-particle collision dynamics simulation technique, we have studied how hydrodynamic interactions affect the stiffening behavior of marginal networks.

We show how the properties of the filaments making up the network, as well as the properties of the solvent it is immersed in, can affect the response of marginal networks to shear. We find that the network is less stiff when hydrodynamic interactions are present than when they are not. The network shear modulus scales as $G' \sim \omega^{\alpha_c}$, with a critical stiffening exponent α_c that can be controlled by varying the network concentration relative to that of the solvent. Our results show that this behavior arises due to the solvent aiding the relaxation of the network and suppressing the network non-affinity, with the system deforming more affinely when hydrodynamic interactions are maximized. Finally, we show how thermal fluctuations can suppress this observed stiffening behavior.

CPP 36.4 Wed 10:45 H47

Rheology of weakly attractive systems: the role of energy dissipation — •Ehsan Irani[1], Pinaki Chaudhuri[2], and Claus Heussinger[1] — [1]Institute for Theoretical Physics, Georg-August University of Göttingen, Göttingen, Germany — [2]Institute of Mathematical Sciences, Tamil Nadu, India

The rheological response of a particulate system with attractive interactions is studied using different models for the dissipation of energy. In systems with the damping force directed normally to the contact point, attractive interactions result in a finite yield stress, and an isostatic structure emerges below the jamming point with shear bands forming as a consequence of non-monotonic flow curves. On the other hand, tangential damping gives rise to the monotonic flow curves and a viscous flow develops in the overdamped regime. However in that case, decreasing the damping factor introduces the inertial time-scale, leading again to non-monotonic flow curves and inertia-induced shear-banding is observed in the underdamped regime. In both cases, the rheology of the system is expressed in terms of relevant damping time-scales and the ratio of dissipative to elastic forces.

CPP 36.5 Wed 11:00 H47

Transport properties of correlated fluids in confinement

— •Christian Rohwer[1,2] and Matthias Krueger[1,2] — [1]Max Planck Institute for Intelligent Systems, 70569 Stuttgart, Germany — [2]4th Institute for Theoretical Physics, University of Stuttgart, 70569 Stuttgart, Germany

Correlations in confined fluids give rise to a wealth of remarkable phenomena. Several equilibrium phenomena, e.g. the critical (thermal) Casimir forces, have been described theoretically and observed experimentally. However, although certain non-equilibrium aspects of such systems can be probed experimentally or through computer simulations, a clear theoretical understanding for confined, correlated fluids out of equilibrium is still lacking.

In this work we consider a dynamical theoretical model for confined fluids with correlations (e.g. oil-water mixtures near / at the critical point), thereby extending known results for bulk systems. In particular, we investigate the steady state velocity profiles in a sheared near-critical fluid film, in dependence on various parameters (e.g. separation of the plates, bulk correlation length, external fields...). Our approach is based on linear response theory for small shearing velocities, and leads to a self-consistent formulation for the shear rate in the film.

We also address the dependence on the choice of dynamical model, since conservation laws strongly affect dynamical time-scales. Lastly we discuss potential experimental realisations of our model.

15 min. break

CPP 36.6 Wed 11:30 H47

The Gyroid phase in a System of Pear-shaped Particles — Philipp Schönhöfer[1], Matthieu Marechal[1], Klaus Mecke[1], Gerd Schröder-Turk[2], and •Douglas Cleaver[3] — [1]Theoretische Physik I, FAU Erlangen, Germany — [2]School of Engineering and IT, Murdoch University, Australia — [3]Materials and Engineering Research Institute, Sheffield Hallam University, UK

It is established that elongated or flattened mesogens like spherocylinders and oblate discs form liquid crystal phases – like the nematic or smectic phase – in addition to the isotropic fluid and crystalline solid states.

A highly complex liquid crystal phase which can be generated by amphiphiles or block co-polymers is the double gyroid Ia3d cubic phase. A promising system which forms this structure consists of hard pear-shaped particles with suitable aspect ratio and degree of tapering.

Using Molecular Dynamics and Monte Carlo simulations with a generalized Gay-Berne potential, the spontaneous formation of the gyroid phase was reproduced. Additionally a defect-free gyroid with the same number of particles per unit cell as the spontaneously formed phase was generated. We calculate the scattering functions and use Voronoi tesselation to study the geometrical properties of both systems.

The next step is to introduce hard spheres which will take up the role of solvent to model mixtures such as the lipid-water system. With an explicit solvent the system should be complex enough to model most common phenomena in cubic phases yet simple enough to allow us to simulate large systems.

CPP 36.7 Wed 11:45 H47

Critical three-body Casimir interaction — •Hendrik Hobrecht and Alfred Hucht — Fakultät für Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg

It was shown by Burkhardt and Eisenriegler that the critical Casimir interaction between two colloids at $T = T_c$ can be calculated exactly by a conformal mapping in arbitrary dimension d [1]. For the two-dimensional case $d = 2$ Bimonte et al. extended this calculation to arbitrary shaped objects [2], where the form of the interaction potential between two disks is known exactly. Utilizing those concepts we present a calculation which maps the case of two separated two-dimensional disks onto a limiting case of a three-body system, where two particles are in contact and one is free to move. We compare the results of this calculation to Monte Carlo simulations, using a highly efficient cluster algorithm [3].

[1] T. W. Burkhardt and E. Eisenriegler, Phys. Rev. Lett. 74, 3189 (1995).

[2] G. Bimonte et al., Europhys. Lett. 104, 21001 (2013).

[3] H. Hobrecht and A. Hucht, Phys. Rev. E 92, 042315 (2015)

CPP 36.8 Wed 12:00 H47

Defect-mediated melting of two-dimensional colloidal quasicrystals — Miriam Martinsons and •Michael Schmiedeberg — Institut für Theoretische Physik 1, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Quasicrystals are structures that possess long range order but no translational symmetry. Due to additional degrees of freedom in quasicrystals there are properties and phenomena that for quasicrystalline structures significantly differ from their counterpart in periodic crystals.

We study how thermally excited excitations or defects develop in two-dimensional colloidal quasicrystals close to the melting transition. According to an extension of the KTHNY theory [1], the formation and dissociation of pairs of dislocation and disclinations is expected to cause the melting of the quasicrystal. Melting should occur via an intermediate phase termed pentahedratic phase [1].

We use Monte-Carlo and Brownian dynamics simulations to study the melting process of decagonal colloidal quasicrystals. By analyzing the positional and bond-orientational correlation functions during the melting process we reveal an intermediate state with quasi-long ranged orientational order but only short ranged positional order as in the predicted pentahedratic phase. Furthermore, we observe network-like structures composed of defects spanning through defect-free areas as well as a coexistence between the intermediate phase and the fluid.

[1] P. De, R.A. Pelcovits, J. Phys. A 22, 1167 (1989); Phys. Rev. B 38, 5042 (1988).

CPP 36.9 Wed 12:15 H47

Protein phase separation controlled by phosphorylation — •David Zwicker[1,2], Oliver Wüseke[3], Jeffrey B. Woodruff[3], Markus Decker[3], Steffen Jaensch[3], Anne Schwager[3], Anthony A. Hyman[3], and Frank Jülicher[2] — [1]School of Engineering and Applied Sciences, Harvard University — [2]Max Planck Institute for the Physics of Complex Systems, Dresden — [3]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden

Biological cells have to organize their proteins in space and time. Membrane-enclosed compartments, like the nucleus, are one solution to this problem. Recent discoveries show that liquid-like droplets are an alternative organization principle. To understand how phase separation can help cells to organize their proteins in space and time, we investigated the formation of the pericentriolar material (PCM), an integral part of the cell scaffold. We combine the theory of phase separation in the presence of chemical reactions with in vivo and in vitro experiments. Our work suggests that the protein responsible for forming the PCM occurs in two different states: one in which it is soluble in the cytosol and one in which it phase separates. The transition between these two states is regulated by chemical reactions that maintain the system away from thermodynamic equilibrium. This allows the cell to control the nucleation process and the growth dynamics, and thus also the droplet count and size. I will discuss the physical principles of this spatial organization, which are likely important for other cellular compartments and might also be used in technological applications.

CPP 36.10 Wed 12:30 H47

Two and three dimensional shapes of simple three and four junction comb polymers — Marvin Bishop[1], Adam J. Barillas[1], Tylor Borgeson[1], •Robin de Regt[2], and Christian von Ferber[2] — [1]Departments of Computer Science and Mathematics, Manhattan College, NY, USA — [2]Applied Mathematics Research Centre, Coventry University, UK

We redesign and apply a scheme originally proposed by G. Wei [Physica A **222**, 155 (1995)] to produce numerical shape parameters with high precision for arbitrary tree-branched polymers based on their Kirchhoff matrix eigenvalue spectrum. This algorithm and a Monte Carlo growth method on square and triangular lattices are employed to investigate the shapes of ideal three and four junction two dimensional comb polymers. We find that the extrapolated values obtained by all of these methods are in excellent agreement with each other and the available theory. We confirm that polymers with a complete set of interior branches display a more circular (resp. spherical) shape.

CPP 36.11 Wed 12:45 H47

How (classical) density functional theory describes structure in electric double layers — •Andreas Härtel[1], Sela Samin[2], and Rene van Roij[2] — [1]Institute of Physics, Johannes Gutenberg-University Mainz, Germany — [2]Institute for Theoretical Physics, Center for Extreme Matter and Emergent Phenomena, Utrecht University, The Netherlands

Ongoing scientific interest is aimed on the properties and structure of electric double layers (EDLs), which are crucial for capacitive water treatment and energy harvesting technologies like desalination devices, blue engines, and thermocapacitive heat-to-current converters. A promising tool for their microscopic description is (classical) density functional theory, which we have applied in order to analyze pair correlations and charge ordering in the primitive model of charged hard spheres. Interestingly, this simple model already describes structural in-plane transitions of EDLs, which occur while their corresponding electrodes are charged. Furthermore, our results demonstrate the impact of screening by solvents on the ability of EDLs to adsorb charges. In conclusion, our work points up issues in the theoretical description of EDLs, which finally might lead to a more sophisticated theory for ionic systems.

CPP 37: Organic-Inorganic Systems II: Energy Level Alignment (organized by O)

Time: Wednesday 10:30–13:00 Location: S054

Invited Talk CPP 37.1 Wed 10:30 S054

Energy level alignment mechanisms at hybrid inorganic/organic semiconductor interfaces — •Norbert Koch — Humboldt-Universität zu Berlin, Berlin, Germany — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

Understanding the energy level alignment at hybrid inorganic/organic semiconductor interfaces is indispensable to devise methods that allow for level control. This is needed to achieve a desired functionality of that heterostructure, as for instance, a type-II alignment facilitates charge separation while a type-I alignment is suitable for energy transfer and radiative recombination. For the inorganic semiconductors ZnO and GaN, the use of interlayers, based on strong molecular acceptors and donors, can be employed to tune the energy level alignment with respect to an organic semiconductor deposited on top. Depending on the level alignment achieved in this way, the hybrid heterostructure functionality, e.g., energy or charge transfer, can be selected. Finally, the impact of the doping level of the semiconductors on interface energetics is discussed for a prototypical hybrid p-n-junction.

CPP 37.2 Wed 11:00 S054

Work Function Increase of GaN and the Influence of Surface Gap States — •Thorsten Schultz[1], Raphael Schlesinger[1], Jens Niederhausen[1,2], and Norbert Koch[1,2] — [1]Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, 12489 Berlin, Germany

The two molecular organic acceptors HATCN and F6-TCNNQ were vacuum-deposited on non-intentionally doped GaN (0001), which had a residual donor concentration of 1016 cm-3. By means of ultraviolet photoelectron spectroscopy, a huge work function increase (up to 1.5 eV for HATCN and 1.7 eV for F6-TCNNQ) was observed for monolayer coverage, which stems mostly from an interface dipole between substrate and molecules. The contribution of band bending within GaN (ca. 0.35 eV, as determined from X-ray photoelectron spectroscopy) was found to be significantly smaller than expected from theoretical calculations that predict the contribution of band bending to be dominating for low doping concentrations. A qualitative model is introduced, which assigns the low band bending contribution to the presence of substrate surface gap states. These states donate electrons to the acceptor molecules, so less charge is transferred from the GaN donors. This results in less band bending change than expected from calculations, which did not take surface states into account. Our investigations show that the energy level tuning scheme via acceptor interlayers, already successfully employed for ZnO, holds great promise for GaN as well.

CPP 37.3 Wed 11:15 S054

Structure and stoichiometry prediction of zinc oxide surfaces — •Philipp Herrmann, Navid Abedi Khaledi, and Georg Heimel — Institut für Physik, Humboldt Universität zu Berlin, Germany

Despite their great potential as transparent electrodes in organic electronics and as integral, active components in hybrid (opto-)electronic devices, full control over the surfaces of transition-metal oxides has remained elusive. Atomistic details of their structure and stoichiometry have proven hard to assess, rendering application-relevant surface properties, such as the work function, highly dependent on environment and preparation conditions.

Here, on the example of zinc oxide, I will present a revised approach to the *ab-initio* prediction of atomistic surface structure and stoichiometry as a function of environmental conditions, specifically temperature and atmospheric composition. The predicted structures will be discussed in terms of their experimental signatures in photoelectron spectroscopy, notably surface core-level shifts and work function.

This work thus paves the way for the targeted *in-silico* design of functional inorganic/organic hybrid interfaces.

CPP 37.4 Wed 11:30 S054

Density-Matrix Derived van der Waals Interactions: Many-Body Dispersion goes Mesoscale — •Martin Stöhr[1,2], Georg Michelitsch[1], John Tully[2], Karsten Reuter[1], and Reinhard Maurer[2] — [1]Technische Universität München — [2]Yale University

The applicability of highly accurate quantum chemical simulation methods is limited to systems of small to moderate size. Density-Functional Theory (DFT), but also more approximate, semi-empirical methods such as Density-Functional based Tight-Binding (DFTB) have shown great success in addressing systems at longer time and length scales. However, a severe drawback of DFTB and many prevalent DFT functionals is the neglect of dispersion interactions, which is particularly consequential for the simulation of e.g. hybrid inorganic-organic systems. Here, we propose a novel approach to obtain effective C6 coefficients in the context of the Tkatchenko-Scheffler dispersion correction scheme [1]. The modified scheme derives atomic dispersion parameters directly from the density-matrix and is thus readily applicable to both full DFT and semi-empirical methods like DFTB, where the electron density is not explicitly constructed. At a fraction of the computational workload of a density-based approach, the scheme yields equally accurate dispersion energies up to the many-body dispersion level for intermolecular interactions in gas-phase and molecular crystals. We exemplify the robustness of the scheme by addressing organic-inorganic interfaces with DFTB using a minimal basis set. [1] A. Tkatchenko and M. Scheffler, *Phys. Rev. Lett.* **102**, 073005 (2009).

CPP 37.5 Wed 11:45 S054

Single molecules of Sexiphenyl on In2O3(111) — •Margareta Wagner[1], Michael Hollerer[2], Martin Sterrer[2], Michael Ramsey[2], Lynn A. Boatner[3], Michael Schmid[1], and Ulrike Diebold[1] — [1]Institut für Angewandte Physik, TU Wien, Österreich — [2]Institut für Physik, Karl-Franzens-Universität Graz, Österreich — [3]Material Science and Technology Division, ORNL, USA

Indium oxide is one of the most important transparent conductive oxides (TCOs), and commonly used as a contact material. Sexiphenyl (6P) is a rod-like molecule and twice as long as the substrate surface lattice parameter of the (111) surface of In2O3 single crystals.

Here, the adsorption of 6P is investigated with STM. We show that 6P has a specific adsorption site, but no well-ordered monolayer is formed. In empty states STM, the single 6P appears as a zig-zag line at bias voltages below +2V. At +2V the molecule starts to appear straight, which is associated with tunneling into the LUMO state. At +2.7V the apparent shape changes again into two bright features, corresponding to the LUMO+1.

CPP 37.6 Wed 12:00 S054

Optical transition energies of isolated molecular monomers and weakly interacting 2D aggregates — Roman Forker[1], Thomas Dienel[2], Andreas Krause[3], •Marco Gruenewald[1], Matthias Meissner[1], Tino Kirchhuebel[1], Oliver Gröning[2], and Torsten Fritz[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — [2]Nanotech@surfaces Laboratory, EMPA - Swiss Federal Laboratories for Materials Science and Technology, Ueberlandstrasse 129, 8600 Duebendorf, Switzerland — [3]NaMLab gGmbH, Noethnitzer Str. 64, 01187 Dresden, Germany

We analyze the $S_0 \rightarrow S_1$ fundamental transition energies observed for 3,4,9,10-perylene tetracarboxylic dianhydride (PTCDA) as a function of coverage on various surfaces with substantially dissimilar dielectric properties. Surprisingly, only two different spectral positions are found: (i) PTCDA$_{\mathrm{HE}}$ basically mimics the behavior of isolated monomers on the surface, while (ii) PTCDA$_{\mathrm{LE}}$, red-shifted by approx. 70 meV, is attributed to a densely packed monolayer (ML) in a two-dimensional herringbone arrangement. This red-shift is in remarkable accordance with previous investigations for PTCDA on NaCl(100) and thus likely arises from the same physical effects, namely the formation of 2D excitonic bands and the polarizability of neighboring molecules within the ML. Possible contributions from substrate-induced molecular distortions and chemical interactions are discussed. Contrary to earlier studies, we conclude that the polarizability of the substrate is not the dominant factor responsible for the reported spectral positions.

CPP 37.7 Wed 12:15 S054

Photoemission study of thin films of the singlet fission compound 1,3-Diphenylisobenzofuran — •David Nobis, Janek Rieger, Daniel Niesner, Pedro B. Coto, Michael Thoss, and Thomas Fauster — Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

Singlet fission (SF) is the conversion of an optically excited, high-energy singlet exciton, into two optically dark, long-lived electronic excited triplet states via a spin-allowed process. This process might be used in next generation solar cells to harvest high-energy light. 1,3-Diphenylisobenzofuran (DPIBF) is a prototypical SF molecule, as has been shown by calculations and optical spectroscopy [1,2].

We investigated thin films of DPIBF on SiO$_2$ with UV photoelectron spectroscopy (UPS) and two-photon photoemission (2PPE). The UPS results show the HOMO located 6 eV below the vacuum level, in good agreement with DFT calculations.

The 2PPE spectra show the first singlet state S_1 at 2.8 eV above the HOMO. The triplet state is 1.4 eV lower in energy. Its high, long-lived population is explained by SF in agreement with literature [2].

[1] Schwerin A. F. *et al.*, J. Phys. Chem. A **114** (2010) 1457
[2] Johnson J. C. *et al.*, Phys. Rev. B **132** (2009) 16302

CPP 37.8 Wed 12:30 S054

Two-photon photoemission from tetraphenylporphyrins on Ag(100) — •Andrej Classen, Rebecca Pöschel, Gianluca Di Filippo, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany

Ultrathin films of two different tetraphenylporphyrins (2HTPP and MgTPP) were grown in-situ under UHV-conditions on a well-defined Ag(100) single crystal. The molecules were deposited by evaporation from a home-built Knudsen-cell evaporator. The substrate was kept at room temperature and layer thicknesses range from one monolayer of molecules (1 ML) up to multilayer films (19 ML). We present an investigation of the electronic structure using ultraviolet photoelectron spectroscopy and monochromatic two-photon photoemission (2PPE). The occupied molecular orbitals of 2HTPP and MgTPP were measured using a photon energy of 21.22 eV (HeI-radiation). 2PPE probes the unoccupied molecular orbitals. The combination of both yields a HOMO-LUMO gap of 4.2 eV (MgTPP) and 4.3 eV (2HTPP) in accordance with literature [1]. Taking the measured work function into account, the ionization potential is 5.9 eV (MgTPP) and 6.1 eV (2HTPP) [2]. The electron affinity is 1.7 eV (MgTPP) and 1.8 eV (2HTPP). The 2PPE intensity as a function of photon energy in the range from 3.08 eV to 3.38 eV follows the absorption spectrum (Soret band) of tetraphenylporphyrin.

[1] X. Blase et al., Phys. Rev. B **83**, 115103 (2011)
[2] Y. Nakato et al., Chem. Phys. Lett. **39**, 358 (1976)

CPP 37.9 Wed 12:45 S054

Work function tuning and electrostatic effects: embedded dipoles in aromatic self-assembled monolayers — Swen Schuster[1], Tarek Abu-Husein[2], David A. Egger[3], Iris Hehn[3], Martin Kind[2], Egbert Zojer[3], Andreas Terfort[2], and •Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany — [2]Institut für Anorganische und Analytische Chemie, Universität Frankfurt, 60438 Frankfurt, Germany — [3]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, 8010 Graz, Austria

Self-assembled monolayers (SAMs) are frequently used as intermediate films to modify charge-carrier injection from metal-electrodes into an organic semiconductor. This is usually achieved by use of the terminal dipolar groups comprising the SAM-ambient interface, affecting, however, the growth chemistry of the semiconductor. Here we suggest an alternative approach, viz. embedding dipolar element into the molecular backbone, decoupling the dipole control and the chemistry at the SAM-ambience interface. In this context, using a representative model system, we studied electronic and structural properties of aromatic SAMs that contain an embedded, dipolar group, viz. pyrimidine. Using a number of complementary characterization techniques combined with quantum-mechanical modeling, we show that such mid-chain substituted monolayers are highly interesting from both fundamental and application viewpoints, as the dipolar groups induce a potential discontinuity inside the monolayer, electrostatically shifting the energy levels in the regions above and below the dipoles relative to one another.

CPP 38: Organic Photovoltaics and Electronics (joint session CPP/HL, organized by HL)

Time: Wednesday 14:45–18:30 Location: H2

Invited Talk CPP 38.1 Wed 14:45 H2

Ultrafast excitonic and charge transfer dynamics in nanostructured organic polymer materials — •Irene Burghardt[1], Robert Binder[1], Matthias Polkehn[1], and Hiroyuki Tamura[2] — [1]Institute for Physical and Theoretical Chemistry, Goethe University Frankfurt, Germany — [2]WPI-Advanced Institute for Material Research, Tohoku University, Japan

We present first-principles quantum dynamical studies of ultrafast photoinduced exciton migration and dissociation in functional organic materials, in view of understanding the key microscopic factors that lead to efficient charge generation in photovoltaics applications. The talk will specifically address (i) exciton dissociation and free-carrier generation in donor-acceptor materials, including models for P3HT-PCBM heterojunctions [1] as well as highly ordered thiophene-perylene diimide assemblies [2], (ii) exciton migration [3] and formation of charge-transfer excitons in oligothiophene H-aggregates, and (iii) exciton multiplication by singlet fission in acene materials [4]. Special emphasis is placed on the critical role of exciton and charge delocalization which are a sensitive function of molecular packing.

[1] H. Tamura, I. Burghardt, J. Am. Chem. Soc. 135, 16364 (2013), M. Huix-Rotllant, H. Tamura, I. Burghardt, J. Phys. Chem. Lett. 6, 1702 (2015). [2] T. Roland et al., Phys. Chem. Chem. Phys. 14, 273 (2012), J. Wenzel, A. Dreuw, I. Burghardt, Phys. Chem. Chem. Phys. 15, 11704 (2013). [3] J. Wahl, R. Binder, I. Burghardt, Comput. Theor. Chem. 1040, 167 (2014). [4] H. Tamura et al., Phys. Rev. Lett. 115, 107401 (2015).

CPP 38.2 Wed 15:15 H2

Non-Equilibrium Charge Carrier Dynamics in Organic Disordered Semiconductors — •Andreas Hofacker[1], Jan Oliver Oelerich[2], Alexey Nenashev[3], Florian Gebhard[2], and Sergei Baranovskii[2] — [1]Institute of Applied Photophysics, Dresden University of Technology, D-01069 Dresden — [2]Department of Physics and Materials Science Center, Philipps-University, D-35032 Marburg — [3]Institute of Semiconductor Physics, 630090 Novosibirsk, Russia

Time-dependent processes in organic semiconductors dominated by non-equilibrium physics are subject of current debate in the scientific community. The understanding of these processes promises fundamental insights into transport and recombination dynamics of charge carriers in organic semiconductor devices such as organic solar cells, and can therefore reveal possibilities for further efficiency enhancement.

Based on an analytical model developed for inorganic disordered semiconductors by Orenstein and Kastner in 1981, we formulate a description of carrier thermalization and recombination in organic disordered semiconductors. For this purpose we extend the very transparent approach of Orenstein and Kastner to enable the description of low recombination rates and applicability of the approach to arbitrary density of tail states (DOS) functions. We predict that the behavior of systems with a Gaussian DOS, which organic semiconductors are commonly believed to be, is distinctively different from systems with an exponential DOS. This fact could be used to experimentally distinguish whether a given sample possesses an exponential or a Gaussian DOS by performing a time-dependent carrier density measurement.

CPP 38.3 Wed 15:30 H2

Mobility-limited recombination models for organic solar cells — •Alexander Wagenpfahl and Carsten Deibel — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

Recent results of kinetic Monte Carlo simulations indicate that recombination of charge carriers in organic semiconductor blends show a strong dependence on the domain size of neat material phases [1]. Consequently, the Langevin recombination model does not generally apply and has to be modified by the geometric mean of the charge carrier mobilities. Here, we present drift–diffusion simulations to reveal the influence of such a recombination model in comparison to the Langevin theory. We discuss differences in the quality of the solar cell current–voltage characteristics and distinguish the different processes which lead to a reduction of the observed recombination rate [2].

[1] Phys. Rev. Lett. 114, 136602 (2015)
[2] Phys. Rev. B 80, 075203 (2009)

CPP 38.4 Wed 15:45 H2

Energy-Gap Law of Non-Radiative Voltage Losses in Organic Solar Cells — •Johannes Benduhn[1], Kristofer Tvingstedt[2], Fortunato Piersimoni[3], Olaf Zeika[1], Donato Spoltore[1], Dieter Neher[3], and Koen Vandewal[1] — [1]IAPP, TU Dresden, Germany — [2]EP VI, Julius-Maximillian University of Würzburg, Germany — [3]IPA, University of Potsdam, Germany

The open-circuit voltage of organic solar cells is low as compared to their optical gap, indicating large energy losses per absorbed photon. These losses arise from the necessity of an electron transfer from an electron donor to an electron acceptor to dissociate the excitons, and furthermore from the recombination of the resulting free charge carriers. It has been shown that the energy loss in the electron transfer event can be below 0.1 eV, while radiative recombination losses are in principle unavoidable.

In this work, we investigate the remaining voltage losses due to non-radiative decay of charge carriers. We find that the non-radiative voltage losses increase when the energy difference between charge transfer (CT) state and ground state decreases. This behaviour is consistent with the "energy gap law for non-radiative transitions", which implies that internal conversion from CT state to ground state is facilitated by molecular vibrations. With this work, we identify a possibly intrinsic loss mechanism, which until now has not been thoroughly considered for organic photovoltaics, and which is different in its very nature as compared to the commonly considered inorganic photovoltaic loss mechanisms of defect, surface, and Auger recombination.

CPP 38.5 Wed 16:00 H2

Development of a photocapacitor based on printed solar cells and supercapacitors — •Katrin Anneser[1], Lukas Hörlin[2], Stephan Braxmeier[1], Andreas Baumann[1], Gudrun Reichenauer[1], and Vladimir Dyakonov[1,2] — [1]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg — [2]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

The main drawbacks of renewable energy sources such as wind and solar energy are unpredictable power fluctuations presenting a major challenge to stability and efficiency of the grid. With increasing fraction of these intermittent energy sources it is necessary to smooth the power before feeding it into the grid without just cutting off the fluctuations. We are following the few previous research activities aiming at combining a fast energy storage device, a supercapacitor, and a solar cell. Rather than developing a modular system our objective is an integrated layered system provided by printing the components from solution processed precursors. Those combined cells will provide a more constant power output compared to stand-alone photovoltaic systems and thus allow feeding into storage units with far slower kinetics (e.g. batteries) or the grid. We present the concept and the related boundary conditions and problems to be solved. Furthermore, we show experimental data from solar cells measured at a high frequency (every second) and derive the basic requirements in terms of power and energy density required for the storage unit per m^2 of the integrated system from these data.

CPP 38.6 Wed 16:15 H2

Passivation and modification of silicon nanowires towards hybrid solar cells — •Jessica Hänisch[1], Carola Klimm[1], Marc A. Gluba[1], Karsten Hinrichs[2], Iver Lauermann[3], Wolfram Calvet[3], Norbert H. Nickel[1], and Jörg Rappich[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium-Photovoltaik, Berlin, Germany — [2]ISAS e.V. - Leibniz-Institut für Analytische Wissenschaften, Berlin, Germany — [3]BESSY, Berlin, Germany

Hybrid solar cells combine inorganic and organic materials to benefit from both areas, particularly in terms of production costs and material consumption. The inorganic-organic interface needs to be well passivated, especially if nanowires with a high surface area are implemented to enhance light absorption. The silicon nanowires were prepared by metal assisted chemical etching (MACE). The etching procedure leads to surface damaging and thereby generates surface defects. These defects reside in the band gap and act as recombination centers. As a consequence, the amount of collected charge carriers is reduced and therefore, the power conversion efficiency decreases. We applied electropolishing procedures to the silicon surface to minimize the amount of surface defects. Changes in the density of surface defects were directly monitored by in-situ photoluminescence measurements. To preserve the improved surface passivation obtained after the electropolishing process we used (electro-)chemical grafting of small molecules and investigated the surfaces by infrared spectroscopy, x-ray photoelectron spectroscopy and photoluminescence measurements.

30 min. Coffee Break

CPP 38.7 Wed 17:00 H2

Vertical Organic Field-Effect Transistors - Functional Principles and Applications — •Alrun Aline Günther[1], Michael Sawatzki[1], Christoph Hossbach[2], Petr Formánek[3], Daniel Kasemann[1,4], Johannes Widmer[1], Johann W. Bartha[2], and Karl Leo[1,5] — [1]Institut für Angewandte Photophysik, TU Dresden, Germany — [2]Institut für Halbleiter- und Mikrosystemtechnik, TU Dresden, Germany — [3]Leibniz-Institut für Polymerforschung Dresden e.V., Germany — [4]currently: CreaPhys GmbH, Dresden, Germany — [5]Fellow of the Canadian Institute for Advanced Research, Toronto (ON), Canada

Vertical organic field-effect transistors (VOFETs) are a means to overcome the limitations of conventional organic field-effect transistors (OFETs). At present however, they often suffer from two major drawbacks: performance limitation by contact effects and limitation to certain materials and processing techniques, making a controlled shift of parameters such as the transistor threshold voltage difficult. Here, we present p- and n-type VOFETs operating in the accumulation and inversion regimes. By introducing contact doping, we are able to increase the transconductance and On/Off ratio of VOFETs by an order of magnitude. We further show that the realisation of inversion VOFETs is possible and can shift the threshold voltage in a controlled manner, while reducing the Off state current of VOFETs through reduction of the source-drain leakage current.

CPP 38.8 Wed 17:15 H2

Vertical Organic Light Emitting Transistors for Investigation of Charge Transport in VOFETs — •Franz Michael Sawatzki[1], Alrun Günther[1], Duyhai Doan[2], Christoph Hossbach[3], Petr Formánek[4], Daniel Kaseman[1,5], Johannes Widmer[1], Thomas Koprucki[2], and Karl Leo[1,6] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, Germany — [2]Weierstraß-Institut für Angewandte Analysis und Stochastik, Leibniz-Institut im Forschungsverbund Berlin e. V., Germany — [3]Institut für Halbleiter- und Mikrosystemtechnik, Technische Universität Dresden, Germany — [4]Leibniz-Institut für Polymerforschung Dresden e.V., Germany — [5]currently: CreaPhys GmbH, 01257 Dresden, Germany — [6]Fellow of the Canadian Institute for Advanced Research (CIFAR), Toronto, Ontario M5G 1Z8, Canada

The vertical organic field effect transistor (VOFET) offers many technological advantages due to its very short geometric channel length. However, in contrast to the standard lateral organic field effect transistor (OFET), the basic physics and working principles are not yet well known. Here, we compare results regarding the charge transport obtained from simulations with measured charge carrier density distributions. The latter ones are obtained from the light emission of vertical organic light emitting transistors (VOLETs). These devices are a combination of an organic light emitting diode (OLED) and a

VOFET, which allow to locally resolve the current path. We show the dependence of the channel size and geometry on the gate-source voltage, the drain-source voltage, and the source geometry.

CPP 38.9 Wed 17:30 H2

Ultra-High Current Densities in Organic Transistors — •Markus P. Klinger, Axel Fischer, Felix Kaschura, Daniel Kasemann, Johannes Widmer, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr Str. 1, 01069 Dresden

Organic transistors are considered for flat panel or flexible displays, radio identification systems, and sensor arrays. Much effort has been spent to optimize the charge carrier mobility and to reduce the channel length of organic field-effect transistors (OFETs). Likewise, new device concepts have been introduced based on charge transport perpendicular to the substrate utilized in so-called vertical organic transistors. One representative is the high-performing organic permeable-base transistor (OPBT) [1,2]. Here, we show that this device is determined by space-charge limited current (SCLC) in the on-state. Thus, OPBTs can drive as much current as possible for a certain thickness of semiconducting material. Using C_{60} with a low charge carrier mobility of about $0.025\,\mathrm{cm}^2\,\mathrm{V}^{-1}\mathrm{s}^{-1}$ in the vertical direction, current densities of more than $600\,\mathrm{A\,cm}^{-1}$ are reached at voltages below 6 V. This performance can be achieved as the total thickness of the device is in the range of 100 nm. With that, OPBTs can easily outperform OFETs in terms of current per footprint area.

[1] M. P. Klinger et al., Adv. Mater. (2015), 27(47);

[2] A. Fischer et al., Appl. Phys. Lett. (2012), 101, 213303

CPP 38.10 Wed 17:45 H2

Controlling the electronic properties in liquid crystal conjugated small molecules for application in electronics — •Nadine Tchamba Yimga[1], Holger Borchert[1], Peer Kirsch[3], Jürgen Parisi[1], and Elizabeth von Hauff[2] — [1]Department of Physics, University of Oldenburg, Germany — [2]Department of Physics and Astronomy, VU University Amsterdam, The Netherlands — [3]Merck KGaA, Liquid Crystals R&D Chemistry, Germany

Organic semiconductors offer numerous advantages for electronics. However, carrier mobilities in organic semiconductors are generally orders of magnitude lower than in inorganic semiconductors. This is a major bottle neck for device efficiency. The electrical properties are additionally dependent on thin film morphology which is challenging to control in solution deposited films. We studied structure-function relationships in a novel liquid crystal molecule. The molecular films demonstrate phase changes from crystalline to nematic to isotropic phases at temperatures of 140 C, 165 C and 250 C, respectively. We demonstrate the influence of temperature on the structure of solution processed films with cross polarized microscope (CPM) and X-ray diffraction (XRD). Current-voltage measurements and impedance spectroscopy were performed on films annealed to temperatures above the crystalline - nematic phase change and subsequently cooled. The mobility increases from 10^{-4} cm^2 V^{-1} s^{-1} to 10^{-3} cm^2 V^{-1} s^{-1}. We demonstrate that controlled structural manipulation of the film can be used to reduce electronic disorder. These results show the potential of liquid crystal conjugated materials in electronic applications.

CPP 38.11 Wed 18:00 H2

Photodetectors Based on an Anilino Squaraine for Efficient Detection of Light in the 700 nm Region — •Andre Pries[1], Matthias Schulz[2], Arne Lützen[2], Jürgen Parisi[1], and Manuela Schiek[1] — [1]Institute of Physics, Energy and Semiconductor Research Laboratory, Oldenburg, Carl von Ossietzky University, Germany — [2]Kekulé Institute of Organic Chemistry and Biochemistry, Bonn, Rheinische Friedrich-Wilhelms-University, Germany

In this work the squaraine derivative 2,4-bis[4-(N,N-diisobutylamino)-2,6-dihydroxyphenyl] squaraine (SQIB) is analyzed in a conventional bulk-heterojunction photodiode architecture, Glass/ITO/MoO_3/SQIB:PCBM/LiF/Al. This architecture shows a power conversion efficiency of ≈2.5 % and a peak external quantum efficiency (EQE) of ≈50 % at 700 nm, making the device highly sensitive in the red wavelength region. In order to even further increase the EQE a negative bias voltage is used. Next the time-dependent response of the device is measured, to find, e.g. the rise- and fall time. Finally, the bandwidth of the device is determined and the cut-off frequency.

[1] G. Chen et. Al, Optical and electrical properties of a squaraine dye in photovoltaic cells, Applied Physics Letters, Vol. 101, No.8 2012, 083904

[2] M.Binda et. Al, Fast and air stable near-infrared organic detector based on squaraine dyes, Organic Electronics, 2009, Vol. 10, Issue 7, p. 1314-1319

CPP 38.12 Wed 18:15 H2

First results of an implementation of GW of reduced complexity for organic semiconductors — •Saber Gueddida and Dietrich Foerster — LOMA, Université de Bordeaux, France

We have implemented a GW algorithm of reduced complexity (N^3 rather than N^4) for crystals containing N»1 atoms in their unit cell. The main ideas of the algorithm and first results of its implementation will be given. Our code aims at contributing to optimizing organic solar cells by predicting the bands and gaps of their constituents.

CPP 39: Focus: Triplet States in Organic Optoelectronics II

Time: Wednesday 15:00–16:30 Location: H37

Invited Talk CPP 39.1 Wed 15:00 H37

The Nature of the 'Triplet Pair State' in Singlet Exciton Fission. — •Jenny Clark[1], Andrew Musser[2], Chaw Keong Yong[2], and Daniel Polak[1] — [1]University of Sheffield, Hicks Buildling, Hounsfield Road, S3 7RH, Sheffield, United Kingdom — [2]University of Cambridge, J J Thomson Avenue, Cambridge CB3 0HE, United Kingdom

Singlet exciton fission is a process by which the bright singlet (spin-0) exciton spontaneously splits into two triplet (spin-1) excitons. The triplets are initially coupled into an overall singlet state, conserving spin. Over time the triplets lose their correlation and become 'free triplets'. The nature of the intermediate state, which may be described as a correlated (entangled) triplet pair has been the subject of debate.

In this talk, I will discuss our recent work describing the nature of the intermediate triplet-pair state and its fate: how it either (i) separates into free triplets; (ii) emits a photon; (iii) returns to the singlet manifold or (iv) in a suitable blend, undergoes double charge-transfer.

I will talk about two material classes: acenes and polyenes and highlight how their different electronic properties affect the process of singlet exciton fission and its potential to be exploited to enhance solar cell efficiency.

CPP 39.2 Wed 15:30 H37

Triplet state formation in polymer:fullerene bulk heterojunction blends — •Frédéric Laquai — Solar and Photovoltaics Engineering Research Center (SPERC), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Kingdom of Saudi Arabia — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Triplet state formation is currently being discussed as a potential loss channel in state-of-the-art bulk heterojunction organic solar cells. However, the precise mechanism of triplet state formation, the relation between the material's chemical structure, film morphology and triplet state yield, and its impact on device performance is still unknown. Here, we present recent spectroscopic results obtained by a combination of fs-ms broadband transient absorption spectroscopy and multivariate curve resolution (MCR) data analysis on two prototypic low-bandgap donor-acceptor copolymers, namely PCPDTBT and its silicon-substituted analogue PSBTBT, in blends with fullerene as acceptor indicating that not only the respective energy levels, but also the solid-state morphology and interfacial structure of the blends influence triplet state formation. These studies have very recently been extended to other common donor polymers including DPP-based materials and PBDTTT-C blends, two systems for which we observe very high triplet yields and in the latter case also recreation of charges due to fast triplet-triplet annihilation on the ns-ms timescale.

CPP 39.3 Wed 15:45 H37

Quantifying Spin-Dependent Recombination in Organic

Bulk Heterojunction Solar Cells — •Stefan Väth[1], Andreas Sperlich[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

In donor-acceptor (DA) based bulk-heterojunction (BHJ) solar cells, the splitting of singlet excitons at the DA interface is crucially important for charge generation. The reversed process, in which two initially free charge carriers meet at the DA interface and recombine is considered as the main recombination process. The intermediate charge transfer state possesses three triplet and one singlet spin configuration which makes the non-geminate recombination process spin dependent. The role of the spin, however, is under continuous discussion and still not clarified yet.

In our experiments, the influence of spin dependent recombination was investigated for organic BHJ solar cells made of the benchmark material system P3HT:PCBM at real operation conditions. For the first time, we combined electrically detected magnetic resonance (EDMR) with the quantitative technique of open circuit corrected transient charge extraction (OTRACE). Extracting photo generated charges under magnetic resonant conditions compared to non-resonant conditions yields in a spin-dependent contribution to the overall recombination of 0.01 % in this particular solar cell system.

CPP 39.4 Wed 16:00 H37

The Nature of Fluorescence Quenching in Single Conjugated Polymer Chains vs. Mesoscopic Aggregates — •Florian Steiner, Jan Vogelsang, and John M. Lupton — Department of Experimental and Applied Physics, University Regensburg, Germany

The photophysics of isolated chains and a bulk film of conjugated polymers (CP) such as poly(3-hexylthiophene) (P3HT) differ substantially. Most prominently, the fluorescence quantum yield drops by at least one order of magnitude upon the transition from dissolved chains to bulk film. The mechanisms behind these differences however are still not fully understood. Here we show that we can clarify the question of fluorescence quenching in CP by using single-particle spectroscopy techniques which can be applied to single polymer chains as well as to isolated aggregates consisting of many polymer chains. By investigating the photon statistics from one single chain at a time, we show that the fluorescence quenching mechanism in P3HT can be attributed to the efficient formation of long-lived triplet states, which are able to quench the fluorescence of the total chain by singlet-triplet annihilation [1]. By applying solvent vapor annealing we are able to grow aggregates of CP. Subsequent single-aggregate photon correlation spectroscopy identifies additional "dark" states, which are more rapidly formed compared to the triplet state. We attribute these "dark" states evolving in the mesoscopic size regime of P3HT to charge transfer states, which play the main role in the strong quenching of the fluorescence at the transition from the single molecule to the bulk film.

[1] F. Steiner et al., PRL 112, 137402 (2014)

CPP 39.5 Wed 16:15 H37

Triplet and Charge Transfer Excitons in Organic Solar Cells: Influene of Energetics and Morphology — •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

To improve organic solar cells it is necessary to develop a deeper understanding of fundamental processes, such as harvesting of singlet and charge transfer (CT) excitons, but also loss mechanisms like electron back transfer (EBT) reactions to the triplet state. These processes depend on the energy levels of constituting donor and acceptor molecules, on microscopic structure of blends but also on the relative spin orientation of charges carriers within the e-h pair. Here, we use electron paramagnetic resonance (EPR) methods to study several polymer-fullerene blend systems and found remarkable correlations between electrical performance of solar cells and formation of CT and triplet excitons. Combining results of complementary experiments, we offer a physical picture on how pushing up the LUMO level of acceptors or tailoring the blends' morphology may end up in unwanted loss mechanisms in bulk-heterojunction solar cells.

CPP 40: Biomaterials and Biopolymers I (joint session BP/CPP/MM, organized by CPP)

Time: Wednesday 15:00–18:15 Location: H40

CPP 40.1 Wed 15:00 H40

Self-assembled plasma protein nanofibers — •Christian Helbing[1], Tanja Deckert-Gaudig[2], and Klaus D. Jandt[1] — [1]Chair of Materials Science, Department of Materials Science and Technology, Otto Schott Institute of Materials Research (OSIM), Faculty of Physics and Astronomy, Friedrich Schiller University Jena, Jena, Germany — [2]Institute for Photonic Technology, Jena, Germany

Protein nanofibers (PNFs) are promising materials for numerous applications in the field of biomedical engineering. Especially, self-assembled PNFs based on plasma proteins have a high importance due their easy fabrication and high biocompatibility. However, knowledge about the self-assembly mechanism of such PNFs is limited. The aim of the current study is to deepen the understanding of the formation mechanism. We tested the hypotheses that morphology and inner structure of PNF depends on environmental conditions. In this work, we present results of self-assembled PNF structures formed in solution from a plasma protein combination. The observed morphology of the formed PNFs depended strongly on the formation conditions. The structural analysis suggest that a partial denaturation, i.e. a change in the secondary structure, of the plasma proteins is a necessary requirement for the formation of PNFs. The comparison of the secondary structure of the PNFs and the native proteins helps to improve the understanding of the self-assembly mechanism. The current results leads to a better control during the PNF formation.

CPP 40.2 Wed 15:15 H40

Automatically recognizing structural patterns in (bio)polymers — •Michele Ceriotti — École Polytechnique Fédérale de Lausanne

Atomistic simulations have been constantly increasing in accuracy and predictive power over the past decade, and materials and molecules of growing complexity are now amenable to modelling. There is however a dire need for algorithms to analyze the outcome of such simulations, to infer the elementary building blocks and the design principles that link atomic-scale structure and the emergence of meso-scale complex behavior. Here I will show how a probabilistic analysis of molecular motifs (PAMM) algorithm can be used to automatically recognize secondary structure patterns in proteins, and discuss how this approach could be used to identify new hydrogen-bond patterns in situations in which biopolymers are encountered in unusual conditions, such as in non-aqueous mediums or at inorganic interfaces.

Invited Talk CPP 40.3 Wed 15:30 H40

Competing oligonucleotide macromolecules: binding preferences instead of a ménage a trois — •Albrecht Ott — Biologische Experimentalphysik, Universität des Saarlandes, Saarbrücken, Germany

The description of macromolecular recognition is usually reduced to the consideration of molecular pairs. In the simplest descriptions the receptor pairs exhibit a lock and key interaction, which mainly depends on the shape of the molecular recognizers, and this is supposed to lead to a highly specific recognition process. Much more refined and quantitative physical descriptions have been proposed, however, they are again based on pairwise interaction, and we remain far from understanding molecular binding in competition as it occurs in a biological organism. Here we present experiments on DNA macromolecular binding in competition. We identify situations where the binding constant of one DNA strand is highly dependent on the presence of another, very similar competitor. We interpret our findings as the result of an interaction term that leads to a formal equivalent of a Landau phase transition. We present experimental results from in vitro transcription assays that highlight the existence of other non-trivial competitive situations that may act along similar lines.

CPP 40.4 Wed 16:00 H40

Poly(ethylene glycol) films and nanomembranes as flexible platform for humidity sensors and bioengineering — Musammir Khan and •Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

We discuss possible applications of novel poly(ethylene glycol) (PEG) hydrogel films and membranes (PHFs and PHMs). They were fabricated by thermally activated crosslinking of amine- and epoxy-terminated, star-branched PEG oligomers and characterized by tunable thicknesses of 4 - 200 nm. As demonstrated, PHFs and PHMs can be used as highly sensitive elements in humidity sensors and moisture-responsive nanoelectronic devices, relying on resistive transduction technique. Their resistance change by ca. 5.5 orders of the magnitude upon relative humidity variation from 0 to 100%, which is unprecedented response for homogeneous materials. As another representative example, we show that PHFs and PHMs are able to host protein-specific receptors, providing, at the same time, protein-repelling and humidity-responsive matrix with a characteristic mesh size up to 8.4 nm. A noticeable grafting density of the test avidin protein, specifically attached to the biotin moieties coupled to the free amine groups in the PHMs, was achieved, whereas the analogous values for non-specifically adsorbed proteins were lower by a factor of 4-5. The engineering of PHMs with biomolecule-specific receptors and their loading with biomolecules are of potential interest for sensor fabrication and biomedical applications, including tissue engineering and regenerative therapy.

CPP 40.5 Wed 16:15 H40

Dynamic biointerfaces: new generation of cell instructive materials — •Chiara Fedele, Ravichandran H. Kollarigowda, Silvia Cavalli, and Paolo A. Netti — Center for Advanced Biomaterials for Healthcare, Istituto Italiano di Tecnologia, Neaples, Italy

Nowadays the growing interest in tissue engineering and biology for the in vitro control of cell fate has led to the design of dynamically actuable platforms through the implementation of stimuli-responsive materials in order to mimic the continuous remodeling of the extracellular matrix in living systems. Dynamic biointerfaces are conceived in order to be able to modify in a predictable spatiotemporal manner the cell-material crosstalk, overcoming the limitations of static conventional biomaterials. In our work, azobenzene-containing photosensitive polymers (e. g. polymer brushes, thin films, crosslinked free standing polymers) are designed as biomaterials to obtain patterned or reshaping substrates using photolithographic techniques or single laser beam instruments, in some cases even in presence of cells, allowing for a real-time modification of cell behavior.

15 min. break

CPP 40.6 Wed 16:45 H40

Tuning the Morphology of Langmuir Polymer Films through Controlled Relaxations of Non-Equilibrium States — •Renate Reiter, Sivasurender Chandran, and Günter Reiter — University of Freiburg, Experimental Polymer Physics, Freiburg, Germany

In general it is difficult to reproduce well defined morphologies of Langmuir polymer films (LPFs) because they have a high propensity to form non-equilibrium states. When these films are allowed to relax, a decay of the surface pressure with time might be observed indicating that the system is not equilibrated. Monitoring the temporal evolution of these relaxations and correlating them with snapshots of the corresponding morphologies sheds light on the associated structural reorganisation processes.

We present a systematic study based on different compression protocols designed to allow for relaxations of LPFs under well defined conditions. The homo peptide poly-γ-benzyl-L-glutamate (PBLG) was chosen for this study because it is a well investigated system that represents the relaxational behaviour of rod-like molecules which is expected to show less complexity than coiled polymer molecules. Our results demonstrate that experimentally manipulating the course of relaxations in LPFs has tremendous impact on the ordering of the molecules. Therefore various macroscopic properties of these biological relevant thin films are accessible.

CPP 40.7 Wed 17:00 H40

Impact of Silver Nanoparticles on the mechanical properties of Aquabacterium biofilms — •Yvonne Schmitt[1], Alexandra Grün[1], Dimitri Demeshko[2], Werner Manz[1], and Silke Rathgeber[1,2] — [1]Institute for Natural Sciences, University of Koblenz-Landau, Koblenz, Germany. — [2]Technology Institute for Functional Polymers and Surfaces (tifko) GmbH, Neuwied, Germany.

The antimicrobial properties of silver nanoparticles (AgNP) led to a wide range of applications in consumer products. As a consequence, there is an increasing release of AgNP into aquatic environments. Biofilms, a conglomerate of extracellular DNA, polysaccharides and proteins, play an important role in sediment stabilization in riverine systems. AgNP are supposed to be a continuous source for silver ions (Ag^+) which can bind to functional groups of the biofilm constituents. This might lead to a decrease in the number of possible intermolecular interactions and, thus, reduced stability of the network. An impairment of the sediment stabilization due to enrichment of the AgNP in the biofilms might be detrimental to the whole ecosystem. In this work we studied the mechanical properties of an *A. citratiphilum* biofilm by means of rheology. The bacterium chosen is representative for a numerically dominant group of bacteria in different freshwater habitats. The biofilm was exposed to environmentally relevant concentrations of AgNP. In order to distinguish physical effects, resulting from the presence of the nanoparticles in the biofilms, from chemical effects, due to the activity of Ag^+, we studied biofilms exposed to Ag^+ as reference. We discuss our results in respect to their environmental implications.

CPP 40.8 Wed 17:15 H40

Characterization of the behaviour of amino acids at bioactive calcite interfaces — •Robert Stepić[1], Zlatko Brkljača[1,2], David M. Smith[2,3], and Ana-Sunčana Smith[1,2] — [1]Institute for Theoretical Physics and Excellence Cluster: Engineering of Advanced Materials, FAU Erlangen-Nürnberg, Nägelsbachstraße 49b, Erlangen, 91052, Germany — [2]Rudjer Bošković Institute, Bijenička 54, 10000, Zagreb, Croatia — [3]Center for Computational Chemistry, FAU Erlangen-Nürnberg, Nägelsbachstraße 25, Erlangen, 91052, Germany

The process of crystal growth controlled by biomolecules is known as biomineralization. This type of controlled growth results in crystals with a myriad of interesting properties, useful in a variety of applications. Therefore it is of great importance to gain deeper insights into the mechanistic details of interactions on the bioinorganic interface. For this purpose we present a systematic study of a set of amino acids, the elementary building blocks of peptides and proteins. Our methodology includes fully atomistic molecular dynamics simulations of the interface made of amino acids, water and slabs of calcite. Two different calcite slabs were taken into account, one with the stable (104) face and one with the unstable (001) face, which is associated with crystal growth. Free energies of binding to both surfaces for all the individual amino acids were determined using a series of sampling simulations with biasing potentials. These in turn reveal the importance of charged and polar groups in the interaction with calcite. This work provides reference data which can be helpful in further theoretical and experimental studies of calcite/peptide interfaces.

CPP 40.9 Wed 17:30 H40

Biomimetic Surface Templating of Silica Nanoparticles by Lysine-Leucine Peptide on Au Substrate — •Hao Lu[1], Yeneneh Yimer[2], Rüdiger Berger[1], Mischa Bonn[1], Jim Pfaendtner[2], and Tobias Weidner[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Chemical Engineering University of Washington, Seattle, USA

Fabrication of silica thin films and architectures has led to many applications in electronic and optical devices, cosmetics, and catalysis; recently, bioinspired silica fabrication approaches have attracted great attention because of low production cost and mild, sustainable fabrication methods. We are the first to demonstrate that the biomimetic molecules can also exert control over silica mineralization when bounded to inorganic surfaces. We use amphiphilic helical peptides based on leucine and lysine side chains (LKa14) carrying cysteine terminal groups as linkers, providing stable covalent bond to gold surfaces. Using XPS, VSFG, and AFM, complemented by molecular dynamic simulation, we have investigated the silica mineralization process at the molecular level directly at the surface: In analogy to solution mineralization, the LKa14 peptides on Au tend to assemble into ordered lateral structures, maintain their solution state helical folding and are oriented upright on the surface. The LKa14 peptides nucleate silica nanoparticles at the surface, which then grow into larger, globular structures. This surface mineralization process serves as a well defined model system for lateral protein assembly and biomineralization and is of potential interest for the design of silica-based biomimetic coatings.

CPP 40.10 Wed 17:45 H40

Reaction kinetics and diffusion in cell-free protein synthesis altered in polymer hydrogels — •Julian Thiele[1], Maike M. K.

Hansen[2], David Foschepoth[2], Hans A. Heus[2], and Wilhelm T. S. Huck[2] — [1]Leibniz Institute of Polymer Research Dresden (IPF), Leibniz Research Cluster (LRC) and Department of Nanostructured Materials, Hohe Straße 6, 01069 Dresden, Germany — [2]Radboud University, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen, NL

Despite the viscous and highly crowded interior of a cell and its influence on diffusion and reaction kinetics, in vitro studies on protein synthesis often fail to take into account the density and spatial organization of the cytoplasm.

We mimic the complex cellular environment using a porous hydrogel matrix, and study the effects of macromolecular crowding on gene expression. While gene expression is strongly decreased by macromolecular crowding in conventional dilute bulk solutions, both gene transcription and translation are significantly enhanced 5x and 4x, respectively, when performed in a microscopic hydrogel environment.

These results highlight the need to consider the influence of the physical environment on complex biochemical reactions including macromolecular crowding as well as microscale confinement and spatial organization.

CPP 40.11 Wed 18:00 H40

Protein-protein interactions in crowded lysozyme solutions — •Karin Julius[1], Michael Paulus[1], Julian Schulze[1], Stefanie Roese[1], Metin Tolan[1], and Roland Winter[2] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, 44221 Dortmund — [2]Fakultät Chemie, Technische Universität Dortmund, 44221 Dortmund, Germany

Inside cells, proteins are surrounded by different macromolecules, including proteins themselves, which cover approximately 30% of the available volume. It has been shown that this reduction of free space by macromolecules, the so called crowding effect, has a significant impact on the stability of proteins, rendering them more resistant to temperature or pressure denaturation. However, the influence of crowding on the protein-protein interaction potential that is mediated by the solvent is still unknown. The final goal of this project is the investigation of the pressure dependent interaction potential between proteins in aqueous protein solution as a function of the crowder concentration, mimicking intracellular solution conditions. For this purpose, small-angle x-ray scattering (SAXS) under high hydrostatic pressure will be applied. As we will focus on the effect of crowding, the well characterized model protein lysozyme is used at a concentration of 5 - 10 wt.-% in combination with the macromolecular crowder Ficoll PM 70 and its monomeric subunit sucrose.

CPP 41: Crystallization, Nucleation, Self Assembly II (joint session CPP/DY, organized by CPP)

Time: Wednesday 16:00–18:30 Location: H42

Invited Talk CPP 41.1 Wed 16:00 H42

From holes to drops to toroids: Transcription of surface patterns into 3D-morphologies by dewetting — •Günter Reiter[1], Samer Al Akhrass[2], and Laurant Vonna[3] — [1]Institute of Physics and Freiburg Materials Research Centre, University of Freiburg, 79104 Freiburg, Germany — [2]Université Claude Bernard Lyon 1, Ingénierie des Matèriaux Polymeres (IMP - UMR CNRS 5223), 15 Boulevard Latarjet, 69622 Villeurbanne Cedex, France — [3]Institut de Science des Matériaux de Mulhouse, (IS2M - UMR CNRS 7361), 15, rue Jean Starcky 68057 Mulhouse Cedex, France

Dewetting of thin films is a simple and thus highly convenient process for creating regularly ordered topographical patterns on various length-scales. Here, we present a general pathway, based on dewetting of a thin polymer film, which allows to convert a chemical surface pattern of hexagonally arranged non-wettable circular patches into a sequence of ordered three-dimensional topographies. With increasing thickness of the dewetting film, cylindrical holes, followed by droplets with the shape of a spherical cap and finally toroids were generated. We identified the width w of the rim, where the dewetted fluid was collected, as the crucial parameter which determined the final three-dimensional morphology. Our experiments demonstrate that for a given surface pattern various three-dimensional morphologies can be obtained by simply varying the initial thickness of the thin film.

CPP 41.2 Wed 16:30 H42

Time-resolved characterization of aggregation during printing of thin films — Stephan Pröller[1], Feng Liu[2], Cheng Wang[3], Thomas P. Russell[2], Alexander Hexemer[3], Peter Müller-Buschbaum[4], and •Eva M. Herzig[1] — [1]Technische Universität München, Munich School of Engineering, Lichtenbergstr. 4, 85748 Garching , Germany — [2]Department of Polymer Science and Engineering, University of Massachusetts Amherst, MA 01003 , USA — [3]Lawrence Berkeley National Laboratory, Advanced Light Source Berkeley , CA 94720 , USA — [4]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching , Germany

The nanomorphology can strongly influence the physical properties of thin films. For example, polymer:fullerene mixtures used in the application for organic photovoltaics vary significantly in performance depending on the inner film morphology. Tracking the actual crystallization and aggregation processes on length scales ranging from sub-nanometers to several tens of nanometers reveals how the different growth processes compete with each other leading to the final film morphology.[1] We can track solvent removal, fullerene aggregation and polymer crystallization with time for different exerimental conditions using grazing incidence x-ray scattering revealing fundamental mechanisms of thin film formation. This information correlated with device performance helps to derive design principles for large scale, industrial thin film fabrication.

[1] Pröller et al, Adv. Energy Mater. DOI:10.1002/aenm.201501580

CPP 41.3 Wed 16:45 H42

Following the crystallization in PEDOT:PSS films during printing — Claudia M. Palumbiny[1], Feng Liu[2], Thomas P. Russell[2,3], Alexander Hexemer[4], Cheng Wang[4], and •Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Materials Science Division, LBNL, Berkeley, USA — [3]Department of Polymer Science and Engineering, UMass, Amherst, USA — [4]Advanced Light Source, LBNL, Berkeley, USA

PEDOT:PSS is one of the most promising electrode materials beyond ITO. Printed films of PEDOT:PSS are compared with ethylene glycol (EG)-doped PEDOT:PSS films and films that are treated with EG after printing and annealing, so-called EG-post-treatment. In-situ GIWAXS is used to determine the structure of the molecules in the crystallites during the printing. During film formation, the dependence of different processing conditions on the resulting interchain coupling (characterized by the pi-pi stacking distance), molecular orientation, and crystallite size are determined as a function of film composition. Thus, understanding the film evolution during the printing process allows for directed modification of solutions and printed films for enhanced organic electronic device performance.

15 min. break

CPP 41.4 Wed 17:15 H42

Towards a multiscale study of aggregation of PCPDTBT in presence of a solvent — •Nancy C. Forero-Martinez[1], Tristan Bereau[1], Bjoern Baumeier[2], and Kurt Kremer[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Department of Mathematics and Computer Science and Institute for Complex Molecular Systems, Eindhoven University of Technology,The Netherlands

Conjugated donor-acceptor polymers are excellent candidates as donor materials for organic photo-voltaic devices due to their charge transport properties. In particular, the microstructure of the low-band-gap PCPDTBT polymer is considered to be affected by the change in morphology of side chains and/or by the processing solvents. The performance of PCPDTBT-optimised solar cells is thus intrinsically linked to the initial preparation of the system: out-of-equilibrium conditions influence the equilibrium system. In this work, we perform multiscale simulations to monitor how the initial presence of solvents drives the formation of PCPDTBT aggregates. We propose as a first step a simplified model of the polymer system that takes into account only CPDT monomers, since their crystalline structure is known experimentally. An atomistic description of the potential energy and the corresponding coarse grained representation are used to study the structure and dynamics of CPDT monomers in solution. We intend to characterise the interactions between polymer and solvent to identify the mechanism promoting aggregation.

CPP 41.5 Wed 17:30 H42

Revealing Structure Formation in conjugated polymers such as PCPDTBT by Optical Spectroscopy — •Anna Köhler[1], Christina Scharsich[1], Florian Fischer[2], Kevin Wilma[3], Fabian Panzer[1], Richard Hildner[3], and Sabine Ludwigs[2] — [1]Experimental Physics II, University of Bayreuth, Bayreuth, Germany — [2]IPOC-Functional Polymers, University of Stuttgart, Stuttgart , Germany — [3]Experimental Physics IV, University of Bayreuth, Bayreuth, Germany

There is increasing evidence that the performance of conjugated polymers in organic solar cells is strongly affected by the presence of small crystallites or aggregates. However, short-range order is difficult to detect using structural techniques. Here, we show that optical spectroscopy can be employed to reveal the presence of short-range ordered structured as well as their formation mechanism. We present a comprehensive study of the optical properties as a function of temperature for PCPDTBT in solution and in thin films with two distinct morphologies.[1] Using absorption and photoluminescence spectroscopy as well as Franck-Condon analyses, we show that PCPDTBT in solution undergoes a phase transition (critical temperature: 300 K) from a disordered to a truly aggregated state upon cooling. Comparison is made to the formation of aggregtes in P3HT.[2] The saturation value of aggregates in solution is reached in PCPDTBT thin films at any temperature. In addition, we demonstrate that a low percentage of thermally activated excimer states is present in the films at temperatures above 200 K.

CPP 41.6 Wed 17:45 H42

Comparing molecules and solids across structural and alchemical space — •Sandip De — Laboratory of Computational Science and Modelling, Institute of Materials, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Evaluating the (dis)similarity of crystalline, disordered and molecular compounds is a critical step in the development of algorithms to classify structures, search chemical space for better compounds and materials, and drive the next generation of machine-learning algorithms for predicting the stability and properties of atomic systems. In recent years several strategies have been designed [1-3] to compare atomic coordination environments. In particular, the Smooth Overlap of Atomic Positions has emerged as a natural framework to obtain translation, rotation and permutation-invariant descriptors of atomic environments, driven by the design of various classes of machine-learned inter-atomic potentials. Here we will present few examples showcasing how one can construct a Sketchmap[4-6] representation of databases of both molecular and bulk structures, using (dis)similarity definitions based on such local descriptors that can treat alchemical and structural complexity within a unified framework.

[1] A. P. Bart ok, et al, Phys. Rev. B88, 054104(2013) [2] Ali Sadeghi et al, J. Chem. Phys. 139, 184118 (2013) [3] Sandip De et al, Phys. Rev. Lett. 112, 083401(2014) [4] G. A. Tribello et al,Proc. Acad. Natl. Sci. U.S.A. 109 5196 (2012) [5] M. Ceriotti et al, Proc. Acad. Natl. Sci. U.S.A. 108 13023 (2011) [6] M. Ceriotti et al, J. Chem. Theory Comput. 9 1521 (2013)

CPP 41.7 Wed 18:00 H42

Area confined nucleation and position control by vapor deposition — •Oleg Buller[1], Hong Wang[2], Wenchong Wang[2], Lifeng Chi[2], and Andreas Heuer[1] — [1]Institut für Physikalische Chemie, WWU, Münster — [2]Physikalisches Institut and Center for Nanotechnology, WWU, Münster

Experimentally it is possible that after vapor deposition of organic molecules on surfaces, prepatterned with a regular gold grid, in basically each cell a single nucleus is formed (defects less than 2%) exactly in the center of each grid. This enormous nucleation and position control can be reproduced for different organic molecules. Via combination of kinetic Monte Carlo simulations and analytical calculations a theoretical explanation for this high quality is provided. In this way it is possible to understand, e.g. that the size of the grid and the external flux simultaneously have to be varied in order to stay in the regime of perfect nucleation and position control. A direct comparison between the experimental and theoretical results is presented.

CPP 41.8 Wed 18:15 H42

Coverage dependent nucleation of PTCDI-C_8 studied by AFM and *in situ* real time XRR and GISAXS — •Anton Zykov[1], Sebastian Bommel[2], Christopher Wolf[1], Linus Pithan[1], Christopher Weber[1], Paul Beyer[1], Gonzalo Santoro[3], Stephan V. Roth[2], and Stefan Kowarik[1] — [1]Inst. f. Physik, Humboldt Universität Berlin — [2]Deutsches Elektronen-Synchrotron DESY, Hamburg — [3]Inst. de Ciencia y Tecnología de Polímeros, CSIC, Madrid

Assembly of molecular building blocks into functional nanomaterials is of great importance for devices however it is difficult to follow molecular scale morphology during growth. Here we show that modern synchrotron small angle X-ray scattering (GISAXS) and X-ray reflectivity (XRR) agree with post growth AFM measurements of roughness and island densities of PTCDI-C_8 on silicon oxide, but additionally offer *in situ* and real time capability. We observe interesting differences in the growth of the 1^{st} and 2^{nd} monolayer (ML) such as different molecular adsorption probabilities and a transition of the island shapes. From the scaling of saturation island densities with substrate temperature and growth rate we evaluate ML dependent nucleation energies and critical nucleus sizes. We discuss our results in the framework of nucleation theories and find that 2^{nd} ML nucleation does not proceed in the often applied diffusion limited aggregation regime. This work shows that X-ray techniques are similarly suited for continuously monitoring multilayer growth and unravel intricate details about sub-monolayer growth.

CPP 42: Focus: Multiscale Simulations for Soft Matter: The Challenge of Dynamics (joint session CPP/DY, organized by CPP)

Organizers: Tristian Bereau , Joseph F. Rudzinski, Kurt Kremer (all MPI Polymerforschung, Mainz)

Multiscale simulations have gained increasing interest in soft matter, due to their ability to better reach the many underlying length and timescales spanning these systems. While significant development of coarsegraining methodologies which aim to accurately describe static equilibrium properties has led to a variety of successful applications, obtaining an accurate description of dynamics remains challenging. This focus session aims at bringing together researchers making various contributions to improving the description of dynamics in coarsegrained models, whether providing a theoretical background, improving parametrization protocols, or studying the limits of existing models.

Time: Wednesday 15:00–18:15 Location: H51

CPP 42.1 Wed 15:00 H51

Reactive molecular dynamics simulations of NaOH solutions — •Matti Hellström and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, Germany

Sodium hydroxide (NaOH) is soluble in water up to very high concentrations and has many applications in chemical industry. Still, surprisingly little is known about the structural and dynamical properties of its aqueous solutions. Using a high-dimensional neural network potential for NaOH(aq) based on dispersion corrected density-functional theory calculations, we have performed large-scale molecular dynamics simulations with close to ab initio quality. First results on many different phenomena like ligand exchange, ion clustering and proton transfer as well as their dependence on concentration are presented and discussed.

CPP 42.2 Wed 15:15 H51

Benchmark of a Reparametrized OPLS Force Field for Chlorinated Hydrocarbons Using Molecular Dynamics Simulations — •Zhu Liu, Jakob Timmermann, Karsten Reuter, and Christoph Scheurer — Theoretical Chemistry, Technische Universität München

The dielectric permittivity sensitively reflects the unique microscopic characteristics of a material [1]. To our knowledge no flexible non-polarizable force field for chlorinated hydrocarbons reliably reproduces this important physical property. We address this situation by reparametrizing an OPLS-AA (Optimized Parameters for Liquid Simulations, All-Atom) force field [2] to optimize the description of dynamic and dielectric properties. Specifically, we refitted the torsional potential energy profile and the atomic partial charges for several molecules from this class to match quantum chemical data. We find the new parametrization to yield a range of physical properties (especially the dielectric constant, isothermal compressibility, and thermal expansion coefficient) in excellent agreement with experimental data for a range of chlorinated hydrocarbon solvents, in addition to getting the surface tension and heat capacity at least as well as the original OPLS-AA model.

[1] C.J.F. Böttcher, Theory of Electric Polarization, Vol. I: Dielectrics in Static Fields, Elsevier B.V., Amsterdam (1973).

[2] W.L. Jorgensen *et al.*, Proc. Natl. Acad. Sci. **102**, 6665 (2005).

CPP 42.3 Wed 15:30 H51

Thermodynamics of polymer nematics: particle-based simulations versus mean-field calculations — •Cristina Greco, Kurt Kremer, and Kostas Daoulas — Max Planck Institute for Polymer Research, Mainz, Germany

Conjugated liquid crystalline (LC) polymers have emerged as promising materials for organic electronics. Predicting their large-scale morphology requires the implementation of mesoscale models. The statistical mechanics of such models is often addressed using mean-field (MF) approaches. These have been very successful in polymer physics and are attractive because of their computational efficiency and straightforward description of thermodynamic properties. For LC polymers, however, deviations between MF predictions and experimental results have been reported, e.g. for the molecular weight dependence of the nematic-isotropic transition. The question then arises: are the discrepancies due to the MF approximation or do they reveal fundamental limitations of the model, e.g. transferability?

To address this issue, we consider a model representing polymer nematics as worm-like chains interacting through soft anisotropic potentials and investigate its phase behaviour by (i) MF calculations based on partial enumeration of conformations, (ii) Monte Carlo simulations. In the latter, accurate free energies are obtained via a special thermodynamic integration scheme which avoids thermodynamic singularities. By comparing the results of the two methods, we can evaluate the effect of fluctuations and local correlations on the macroscopic behaviour.

CPP 42.4 Wed 15:45 H51

Comparing atomistic and coarse-grained simulations of P3HT — •Jonathan Gross, Momchil Ivanov, and Wolfhard Janke — ITP Uni Leipzig

Poly(3-hexylthiophene) (P3HT) is a key material used in organic photovoltaics (OPVs). In this study we assess the validity of two coarse-grained models of P3HT. We compare coarse-grained Monte Carlo simulations to fully atomistic molecular dynamics simulations. Structural properties of single polymer chains of short to medium lengths are compared between the three representations.

Invited Talk CPP 42.5 Wed 16:00 H51

A coarse-grained model for DNA: dynamics of self-assembling biological systems and nanostructures. — •Ard Louis — Theoretical Physics, University of Oford

DNA is a particularly promising candidate for large-scale self-assembly because the specific binding of DNA bases can be accurately designed to build dynamic structures on the nanoscale with atomic precision. Inside the cell, DNA not only stores information in a digital code, but controls its readout by subtle modulation of its dynamic properties.

To study processes on these time and length-scales we employ oxDNA[1], a nucleotide level coarse-grained model that can model dynamical DNA structures with thousands of nucleotides. We are able to accurately reproduce the dynamics of exchange reactions, a key component of dynamic DNA nanotechnology, and also make detailed predictions for the hybridization dynamics of DNA duplexes. Larger structures such as a DNA nanobot can also be studied. For the dynamics of large-scale addressable assemblies, we develop a new multi-scale technique. As is the case for many other coarse-grained systems, correctly interpreting dynamical results is subtle[2].

[1] http://dna.phyiscs.ox.ac.uk [2] J.T. Padding and A.A. Louis, Phys, E 74, 031402 (2006)

15 min. break

CPP 42.6 Wed 16:45 H51

Cycle representatives for the coarse-graining of systems driven into a non-equilibrium steady state — •Fabian Knoch and Thomas Speck — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudingerweg 7-9, 55128 Mainz, Germany

A major current challenge in statistical mechanics poses the systematic construction of coarse-grained Markov State Models [1] that are dynamically consistent, and, moreover, might be used for systems driven out of thermal equilibrium. Here we present a novel prescription that extends the Markov state modeling approach to driven systems violating detailed-balance [2]. In more detail, we decompose a given Markov State Model in cycles and introduce the concept of cycle representatives, which stand for many cycles that share similar properties. The coarse-graining involves the renormalization of transition rates that preserves the entropy production of the original Markov State Model. We illustrate our new methodology by an intuitive example: A particle trapped in a 2-dimensional double well potential and driven by a non-conservative force.

[1] Prinz, J.-H., Wu, H., Sarich, M., Keller, B., Senne, M., Held, M., Chodera, J. D., Schütte, C. and Noe, F. Markov models of molecular kinetics: Generation and validation. JCP 134(17), 2011

[2] Knoch, F. and Speck, T. Cycle representatives for the coarse-graining of systems driven into a non-equilibrium steady state. New Journal of Physics 17(11), 2015

CPP 42.7 Wed 17:00 H51

Improving the kinetics from molecular simulations using biased Markov state models — •Joseph Rudzinski, Kurt Kremer, and Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

Molecular simulations can provide microscopic insight into the physical and chemical driving forces of complex molecular processes. Despite continued advancement of simulation methodology, model errors may lead to inconsistencies between simulated and experimentally-measured observables. This work presents a robust and systematic framework for reweighting the ensemble of dynamical paths sampled in a molecular simulation in order to ensure consistency with a set of given kinetic observables. The method employs the well-developed Markov state modeling framework in order to efficiently treat simulated dynamical paths. We demonstrate that, for two distinct coarse-grained peptide models, biasing the Markov state model to reproduce a small number of reference kinetic constraints significantly improves the dynamical properties of the model, while simultaneously refining the static equilibrium properties.

Invited Talk CPP 42.8 Wed 17:15 H51

Principle of Maximum Caliber and its application in biology — •Kingshuk Ghosh — University of Denver

We will describe the principle of Maximum Caliber (MaxCal), a variational approach to model dynamical fluctuations. MaxCal is similar to the Maximum Entropy principle but applied in the trajectory space, natural language in describing several biological systems ranging from macromolecular dynamics to networks. We will briefly describe the general formalism and show the equivalence between MaxCal and Markov processes. Next we will present application of MaxCal to model stochastic dynamics in biological systems, in particular genetic networks. These applications will highlight the role of MaxCal in describing complex systems with cooperativity, non-linearty and feedback in a coarse-grained manner and yet provide us with quantitative tools to analyze data and gain valuable insights.

Invited Talk CPP 42.9 Wed 17:45 H51

Coarse-graining of conservative and non-conservative interactions in molecular liquids — •Nico van der Vegt — Technische Universität Darmstadt, Darmstadt, Germany

In my talk, I will discuss two central challenges in multiscale simulations of soft matter: How can we improve the transferability of bottom-up coarse grained models? How can we improve the coarse-grained model's dynamical properties? Both questions are important, in particular when transport and nonequilibrium processes are studied. I will present a bottom-up coarse-graining procedure for constructing conservative and non-conservative (dissipative and stochastic) interactions for Dissipative Particle Dynamics (DPD) models of molecular liquids. This procedure is based on the Conditional Reversible Work (CRW) method.[1] I will address the chemical and state-point transferability of conservative potentials for coarse-grained molecular liquids in bulk and at interfaces,[2,3] and discuss challenges that remain in modelling dynamical properties of molecular liquids with CRW-DPD models.[4]

References: (1) E. Brini, V. Marcon, N. F. A. van der Vegt, PCCP 13, 10468-10474 (2011). (2) E. Brini, N. F. A. van der Vegt, J. Chem. Phys. 137, 154113 (2012). (3) V. R. Ardham, G. Deichmann, N. F. A. van der Vegt, F. Leroy, J. Chem. Phys. 143, 243135 (2015) (4) G. Deichmann, V. Marcon, N. F. A. van der Vegt, J. Chem. Phys. 141, 224109 (2014)

CPP 43: Poster: The Physics of Water Interactions with Biological Matter

Time: Wednesday 18:15–21:00 Location: Poster B2

CPP 43.1 Wed 18:15 Poster B2

Phase behavior of thermoresponsive polymers in dependence on temperature and pressure — •Kora-Lee Claude[1], Simon Pinzek[1], Konstantinos Kyriakos[1], Anna Miasnikova[2], André Laschewsky[2], Peter Müller-Buschbaum[1], Alfons Schulte[3], and Christine M. Papadakis[1] — [1]Technische Universität München, Physik-Department, Garching, Germany — [2]Universität Potsdam, Institut für Chemie, Germany — [3]University of Central Florida, Department of Physics and College of Optics & Photonics, Orlando, U.S.A.

Thermoresponsive polymers constitute an important class of soft matter. Poly(N-isopropyl acrylamide) (PNIPAM) exhibits lower critical solution temperature (LCST) behaviour in aqueous solution: When heated above the cloud point, the chains release water and collapse, leading to phase separation. As an alternative to temperature variation, the phase transition can also be induced applying high pressure, which offers the possibility to map out p-T-phase diagrams.

In the present work, we use temperature- and pressure-resolved turbidimetry to measure the p-T-phase diagram of PNIPAM in a large range and to determine the involved thermodynamic parameters more precisely. Moreover, block copolymers from polystyrene and PNIPAM as well as a novel thermoresponsive polymer are investigated.

CPP 43.2 Wed 18:15 Poster B2

On the influence of the intermolecular potential on the wetting properties of water on silica surfaces — •Elvira Pafong, Julian Geske, and Barbara Drossel — Institut für Festkörperphysik, Technische Universität Darmstadt

Porous amorphous silica is widely used for technological applications such as catalysators, nanotechnology, or biomedicine. Often, an aqueous solution is given into the pores, and it is therefore essential to understand the structure, dynamics and wetting behavior of water in such nanoporous systems. Due to the ability of water to form hydrogen bonds with the surface silanol groups of the silica material, the surfaces are believed to be highly hydrophilic and the water is expected to wet the pores even at moderate filling ratios. However, this is not seen in our molecular dynamics simulations using the standard Brodka-Zerda form of the Lennard Jones potential. We therefore perform an in-depth study of the effect of the choice of the potential and of the thickness of the silica walls on the behavior of water in partially filled pores and on top of silica slabs. We find that the Gulman potential gives more realistic wetting behavior. We also find that the thickness of the silica slab must be chosen carefully in other to well reproduce the electrostatic and van-der-Waals interactions between water and silica surfaces.

CPP 43.3 Wed 18:15 Poster B2

Molecular dynamics simulations of radon accumulation in water and oil — •Elvira Pafong and Barbara Drossel — Institut für Festkörperphysik, Technische Universität Darmstadt, 64289 Darmstadt

Radon is a radioactive gas that can enter the human body from air or from ground water. Radon can accumulate to levels that considerably rise the risk of lung cancer while it is also known as a a treatment of various ailments, most notably rheumatoid arthritis. The accumulation of radon differs between tissues, with particularly high concentrations in fatty cells. In order to understand the mechanisms responsible for the different solubility of radon in water and fat, we perform molecular dynamics simulations of radon gas at ambient conditions in contact with a bulk material consisting either of water or oil. We evaluate the diffusion coefficient of radon in both media as well as the equilibrium concentration. The crucial point here is to understand the hydrophobic interaction between water and radon as compared to the dispersive interaction between radon and oil. Therefore, we artificially vary the water charges (i.e., the hydrophobicity) as well as the parameters of the van-der-Waals interaction.

CPP 43.4 Wed 18:15 Poster B2

3D-Depth Profiling of Soft and Hydrated Polymeric Surfaces using Atomic Force Microscopy — •Martin Dehnert, Manuel Uhlig, Diana Voigt, and Robert Magerle — Fakultät für Naturwissenschaften, TU Chemnitz, Germany

Tapping mode atomic force microscopy (AFM) is widely used for imaging surfaces of soft materials such as polymers, biological cells, tissues, and even liquids. With tapping mode AFM the shape of the surface (the height image) is measured simultaneously with the phase image from which local mechanical properties of the specimen can be inferred. On soft polymeric materials, however, the tip can indent several tens of nanometers into the surface, which can cause artefacts in both height and phase images. [1] The position of the unperturbed surface and the tip indentation can be determined from point-wise measurements of the amplitude and the phase as function of the tip-sample distance. [1] Furthermore, the tip indentation can be used as depth coordinate for reconstructing three-dimensional depth profiles of the tip-sample interaction. [2] Here, we compare 3D-depth profiles of soft and hydrated polymeric surfaces, for example, polystyrene-functionalized graphene oxide, fluid polymers, and hydrated collagen fibrils by means of dynamic and static force distance measurements. We discuss the different contributions to the tip-sample-interaction and show how the unperturbed surface of compliant materials can be measured.

[1] A. Knoll, R. Magerle, G. Krausch, Macromolecules **34**, 4159 (2001)

[2] E.-C. Spitzner, C. Riesch, R. Magerle, ACS Nano **5**, 315 (2011)

CPP 43.5 Wed 18:15 Poster B2

Water Transport through 1-nm-Thick Functional Carbon Nanomembranes — •Yang Yang[1], Xianghui Zhang[1], Sergey Shishatskiy[2], Jan Wind[2], Volker Abetz[2], André Beyer[1], and Armin Gölzhäuser[1] — [1]Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany — [2]Institute of Polymer Research, Helmholtz-Zentrum Geesthacht, 21502 Geesthacht, Germany

Water transport through two-dimensional materials is fundamentally important for understanding the interactions of water and materials. From an application point of view, membrane thickness plays an essential role in efficient separation since a minimal thickness can minimize the transport resistance and maximize permeate flux. The synthesis of 1-nm-thick functional carbon nanomembranes (CNMs) offers exciting opportunities for enriching our understanding of water interactions as well as for developing a new class of efficient membranes [1]. CNMs are made by electron induced cross-linking of aromatic self-assembled monolayers and can be transferred to almost any surface. Here we present the fabrication of a composite membrane which comprises a CNM top layer and a porous polyacrylonitrile (PAN) support membrane. The membrane thickness, composition and structure were characterized by employing X-ray photoelectron spectroscopy, atomic force microscopy and helium ion microscopy. The water transport through CNMs is investigated in a pressure-driven process and the first permeation results will be presented and discussed.

[1] M. Ai, et al. Carbon Nanomembranes (CNMs) Supported by Polymer: Mechanics and Gas Permeation. Adv. Mater. 2014, 26, 3421

CPP 43.6 Wed 18:15 Poster B2

Specific Effects of Ca^{2+} Ions and Molecular Structure of β-Lactoglobulin Interfacial Layers at Air/Water Interfaces — •Felix Schulze-Zachau and Björn Braunschweig — Institute of Particle Technology (LFG), Friedrich-Alexander University of Erlangen-Nürnberg (FAU), Cauerstrasse 4, 91058 Erlangen, Germany

β-lactoglobulin (BLG) adsorbate layers at air-water interfaces were studied on a molecular level with vibrational sum-frequency generation (SFG), tensiometry and ellipsometry and on a macroscopic level by foam property measurements as a function of bulk Ca^{2+} concentrations (C). For C <10 mM, a strong decrease in SFG intensity of O-H stretching bands from interfacial water molecules is observed. This decrease is indicative of charge screening and presumably also of specific ion interactions. Support for the latter comes from a change in polarity of C-H stretching modes from aromatic amino acid residues such as Trp, accompanied by an abrupt increase in layer thickness from 5 to 10 nm. Such a polarity change was previously observed in a pH dependent study where the isoelectric point of BLG was crossed and is likely to be associated with interfacial charge compensation and overcharging due to the presence of Ca^{2+}. Macroscopic foam stability, however, is decreased once the interfacial charges become fully screened which is in line with previous studies of thin foam films. Once the negative net charge of BLG is overcharged by Ca^{2+} at high C, agglomerates at the interface start to form which increase the layer thickness and interfacial elasticity and decrease the viscosity of the interfacial layer which leads to much higher foam stabilities and smaller bubble sizes.

CPP 43.7 Wed 18:15 Poster B2

Nanoskalige mechanische Eigenschaften hydrierter Kollagenfibrillen — Diana Voigt[1], Manuel Uhlig[1], Martin Dehnert[1], Anke Bernstein[2] und •Robert Magerle[1] — [1]Fakultät für Naturwissenschaften, TU Chemnitz, Chemnitz — [2]Orthopädie und Traumatologie, Universitätsklinikum Freiburg, Freiburg

Faserbildende Kollagene sind ein Hauptbestandteil der Bindegewebe von Wirbeltieren. Die häufigste Art ist Kollagen vom Typ I, das 300 nm lange Tropokollagene bildet, die sich zu Fibrillen mit typischerweise 30 bis 300 nm Durchmesser anordnen, wobei die Fibrillen eine periodische Struktur (die D-Bande) mit 67 nm Wiederholeinheit entlang der Fibrillenachse aufweisen. Die Verteilung von Wassermolekülen innerhalb der Kollagenfibrillen bestimmt entscheidend die mechanischen Eigenschaften der Fibrillen. Wir untersuchen die nanoskaligen mechanischen Eigenschaften hydrierter Kollagenfibrillen mittels Rasterkraftmikroskopie und verschiedenen Arten der Kraftspektroskopie, wobei wir den Wassergehalt der Fibrillen über die Luftfeuchte kontrolliert einstellen können. Das nanoskalige Quellverhalten der Fibrillen gibt direkte Hinweise auf unterschiedliche Mengen von freiem und gebundenem Wasser in den Überlapp- und Lückenbereichen der D-Bande. Ferner können wir räumliche Tiefenprofile der mechanischen Eigenschaften der Kollagenfibrillen rekonstruieren.

CPP 43.8 Wed 18:15 Poster B2

Landau-Ginzburg theory for indirect membrane interactions — •Alexander Schlaich[1], Jan Daldrop[1], Bartosz Kowalik[1], Matej Kanduč[1,2], Emanuel Schneck[3], and Roland R. Netz[1] — [1]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — [2]Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, 14109 Berlin, Germany — [3]Department of Biomaterials, Max Planck Institute of Colloids and Interfaces, 14476 Potsdam, Germany

Hydrophilic interfaces, such as planar lipid membranes, show overwhelming repulsive behavior at nanometer separations in aqueous solution that is not captured within classical continuum theories. It is common consensus that the atomistic degrees of freedom need to be considered explicitly. Marcelja and Radic were the first to propose that water orientation causes a significant contribution to the interaction free energy.

Using field-theoretical modeling, we derive the phenomenological interaction parameters for a Landau-Ginzburg model and show that employing the water dipole orientation we can quantitatively describe the indirect interaction between surfaces, i.e. the contribution of water acting on a single surface.

CPP 43.9 Wed 18:15 Poster B2

The local structure in concentrated yttrium(III) chloride aqueous solutions under high hydrostatic pressure — •Mirko Elbers[1], Karin Julius[1], Michael Paulus[1], Christian Sternemann[1], Florian Wirkert[1], Julia Nase[1], Paul Salmen[1], Göran Surmeier[1], Ralph Wagner[2], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, TU Dortmund, Germany — [2]Fachbereich C - Physik, Bergische Universität Wuppertal, Germany

We present an extended X-ray absorption fine structure (EXAFS) study on the hydration properties of yttrium(III) chloride (YCl_3) under high hydrostatic pressures. In order to take a closer look at ion-ion interactions, aqueous salt solutions with different concentrations were investigated. In nature, the interaction between macromolecules or nanoparticles is mediated by the surrounding aqueous phase. Thus, changes in the water structure, e.g. by the application of pressure or the addition of ions, have a direct impact on the particle-particle interaction potential. For example, in a pressure dependent small angle X-ray scattering study of dense aqueous lysozyme solutions, we found a minimum of the attractive interaction strength at a hydrostatic pressure of 2 kbar. This effect was assigned to a collapse of the second hydration shell of the surrounding water, which might be affected by the addition of ions. Hence, we studied the pressure dependence of the local structure of salt solutions by EXAFS measurements between 1 bar and 5 kbar at concentrations of up to 3M. Furthermore, we performed additional molecular dynamics (MD) simulations of the investigated sample system to interpret the experimental data.

CPP 43.10 Wed 18:15 Poster B2

Lower critical solution temperature behaviour in protein solutions caused by cation-induced hydration effects — •Olga Matsarskaia[1], Michal Braun[1], Felix Roosen-Runge[2], Marcell Wolf[1], Roland Roth[3], Fajun Zhang[1], 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

Upper and lower critical solution temperatures (UCST / LCST) are well known in systems such as mixtures of organic liquids. Here, we demonstrate for the first time an LCST in an aqueous protein (bovine serum albumin, BSA) solution which is induced by trivalent metal cations such as Y^{3+}. The LCST manifests itself as a liquid-liquid phase separation (LLPS) above a certain temperature. Supported by calorimetric data, in their contribution we rationalise the mechanism behind this new case of LCST as follows. It is known from crystal structures that the Y^{3+} cations bind to negatively charged carboxyl groups of acidic residues on the protein surface and can bridge protein molecules [1]. Both Y^{3+} and carboxyl groups are strongly hydrated. For protein-cation binding to occur, both binding partners need to shed their hydration shells. Hydration water molecules are thus released into bulk water, increasing the entropy of the system. With increasing temperature, this entropy-driven binding process becomes more efficient, inducing a short-range attraction into the system which ultimately leads to LLPS.

[1] Zhang et al. (2011). J. Appl. Cryst., 44, 755.

CPP 43.11 Wed 18:15 Poster B2

Tracer diffusion in heterogeneous environments: Towards analytic fit functions — •Felix Roosen-Runge, Dominique Bicout, and Jean-Louis Barrat — Institut Laue-Langevin, Grenoble, France

Tracer diffusion in heterogeneous environments is a relevant and frequently studied phenomenon in experiment, simulation and theory. A paradigmatic example is water diffusion through hydration shells around biomacromolecules or membranes. Analytical fit functions for complex systems such as these are rare, although they would be an interesting means to connect conceptual ideas to experimental results. We report on an approach to recover effects of geometry and position-dependent diffusivity by approximate solutions well-suited for data fitting. We derive an analytical function for an isotropic motion switching between different diffusive states, and extend the approach towards anisotropic systems such as layer structures. Finally, we discuss the challenges, limitations and potentials of the outlined method for data analysis integrating experimental and theoretical knowledge.

CPP 44: Poster: Biomaterials and Biopolymers

Time: Wednesday 18:15–21:00 Location: Poster B2

CPP 44.1 Wed 18:15 Poster B2

Macromolecular HPMA-Based drug delivery system - behavior in protein environment — •Xiaohan Zhang[1], Bart-Jan Niebuur[1], Petr Chytil[2], Tomas Etrych[2], Sergey K. Filippov[2], Alexey Kikhney[3], Florian Wieland[3], Dmitri I. Svergun[3], and Christine M. Papadakis[1] — [1]Technische Universität München, Physik-Department, Fachgebiet Physik weicher Materie, Garching, Germany — [2]Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Prague, Czech Republic — [3]European Molecular Biology Laboratory, DESY, Hamburg, Germany

Polymer drug carriers based on N-(2-Hydroxypropyl)methacrylamide (HPMA) copolymers bearing cholesterol moieties have been studied extensively over the past few years, to understand the aggregation behavior and shape of the copolymers in dilute aqueous solutions [1,2]. Above certain concentration, micelle-like nanoparticles (NPs) having ellipsoidal shape are observed. However, there is a lack of knowledge on the behavior of these drug carriers in human blood environment.

We use fluorescence life-time correlation spectroscopy (FLCS) and small angle X-ray scattering (SAXS) to investigate HPMA copolymers that are dissolved in an aqueous solution of human serum albumin (HSA) to reveal the interaction between the NPs and HSA. The size of the NPs is reduced when HSA is present. We suspect that some of the cholesterol moieties bind to HSA and are removed from the nanoparticles.

[1] S. K. Filippov, et al., Biomacromolecules, 2012, 13, 2594

[2] S. K. Filippov, et al., Biomacromolecules, 2013, 14, 4061

CPP 44.2 Wed 18:15 Poster B2

Fabrication and Analysis of graphene quantum dots synthesized by the Electrolysis of Graphite — •Sonja Allani, Stefan Fasbender, and Thomas Heinzel — Heinrich Heine Universität Düsseldorf

Fluorescent graphene quantum dots (GQDs) are prepared by the electrolysis of graphite rods in aqueous solution of NaOH and subsequent treatment with hydrazine hydrate. The method described by Zhang et al. [1] is modified and the influence of the synthesis parameters on the GQDs fluorescence and size is investigated. In order to sort the GQDs by size, dialysis with different membrane pore sizes is realized. Dialysis is also used to obtain a pure GQD solution of pH = 7, providing the opportunity for future use in bioimaging applications. Fluorescence and absorbance spectra are taken and Atomic Force Microscopy is used to determine the GQDs size and shape.

[1] Zhang et al., J. Mater. Chem., 2012, 22, 7461-7467

CPP 44.3 Wed 18:15 Poster B2

Ab initio molecular dynamics simulations of intramolecular hydrogen bonds in low molecular weight polyethylene glycol — •Mariana Kozlowska and Pawel Rodziewicz — University of Bialystok, Ciolkowskiego Str. 1K, 15-245 Bialystok, Poland

Polyethylene glycol (PEG) is an amphiphilic polyol with a wide range of applications in medical, chemical and biological areas. Its structural properties were previously investigated theoretically utilizing classical molecular dynamics simulations. Such studies, however, have not taken the possibility of the formation of intramolecular hydrogen bonds into consideration.

In this work, we use static DFT calculations to analyze in detail intramolecular hydrogen bonds formed in the low molecular weight PEG with two to five repeat subunits. Both red- (O-H...O) and blue-shifting (C-H...O) H-bonds, which control the structural flexibility of PEG, are analyzed. The existence and the strength of intramolecular H-bonds is analyzed utilizing the Quantum Theory of Atoms in Molecule. Car-Parrinello molecular dynamics simulations are used to mimic the structural rearrangements and the H-bond breaking/formation in the PEG molecule at 300 K.

The authors gratefully acknowledge the financial support of the University of Bialystok within the Grant for Research of Young Scientists, grant number BMN 175.

CPP 44.4 Wed 18:15 Poster B2

Fluorescence properties of Graphene Quantum Dots and Graphene Oxide derived by the thermolysis of citric acid — •Christian Wimmenauer, Stefan Fasbender, and Thomas Heinzel — Heinrich Heine Universität Düsseldorf

Fluorescent graphene quantum dots (GQDs) and graphene oxide (GO) are prepared by thermal decomposition of citric acid. The influence of different heating temperatures and different durations of the thermolysis on the fluorescence properties of GQDs and GO are investigated and a sharp distinction in the absorbance spectra of GQDs and GO is observed. Atomic Force Microscopy is used to determine the GQDs size and shape and the GQDs are sorted by size using dialysis membranes with different membrane pore sizes. Dialysis in deionized water is realized to obtain a pure aqueous GQD solution of pH = 7, allowing the possible use in bioimaging applications.

CPP 44.5 Wed 18:15 Poster B2

Three-dimensional microstructures on flexible substrates fabricated by two-photon polymerization for use as cell substrates and for wetting experiments — •Cristina Plamadeala[1], Johannes Heitz[1], Jaroslaw Jacak[1], Gerda Buchberger[2], Werner Baumgartner[2], Birte Magnus[3], and Rainer Marksteiner[3] — [1]Institute of Applied Physics, Johannes Kepler University Linz, Austria — [2]Innovacell Biotechnologie AG, Innsbruck, Austria — [3]Institute of Biomedical Mechatronics, Johannes Kepler University Linz, Austria

Polymer microstructures with various geometries are written onto a flexible substrate by the technique of two-photon polymerization by a Ti-sapphire femtosecond-laser, which is focused into a liquid acrylate based resin containing a photo-initiator. The microstructures are employed either as three-dimensional tissue scaffold onto which adherent cells can be seeded or are used as topological substrates for wetting experiments. Due to confinement to the microstructures and/or mechanical interaction with the scaffold, the cells are stimulated to grow three-dimensionally and to produce calcium binding proteins. There are some similarities in the way the microstructures are filled by cells and by water in wetting tests. Beyond the use of cell scaffolds, the structures may therefore have other potential applications in the field of microfluidics due to their good wettability and water sustainment.

CPP 44.6 Wed 18:15 Poster B2

Raman spectroscopic investigation of tannin-furanic rigid foams — Andreas Reyer[1], Gianluca Tondi[2], Raphael Berger[1], Alexander Petutschnigg[2], and •Maurizio Musso[1] — [1]Fachbereich Chemie und Physik der Materialien, Universität Salzburg, Hellbrunnerstrasse 34, 5020 Salzburg, Österreich — [2]Fachhochschule Salzburg Campus Kuchl, Markt 136a, 5431 Kuchl, Österreich

Tannin-furanic rigid foams are innovative polymeric materials made of inexpensive organic ingredients, and are usually produced via an acid catalyzed polycondensation reaction between furfuryl alcohol and condensed flavonoids (e.g. Mimosa tannin). These bio-friendly foams have already been proposed e.g. as insulating material for eco-sustainable buildings (green building technology), their most important physical properties being their low thermal conductivity and their high fire resistance. The target of the present study is the Raman spectroscopic characterization of the tannin-furanic rigid foams in order to compare their spectral signature with that of the precursor materials furfuryl alcohol, polymerized furfuryl alcohol, and Mimosa tannin, by means of multi-wavelength Raman spectroscopy (at 1064 nm, 532 nm, and 455 nm laser excitation), thereby including a comparison with infrared spectra reported in recent literature, and a discussion on similarities and differences to the spectral signatures of polymer-like sp2 carbon-based materials, and on the the still preserved organic nature of the tannin-furanic foam.

CPP 44.7 Wed 18:15 Poster B2

rubber elasticity for percolation network consisting of gaussian chains — •kengo nishi[1], mitsuhiro shibayama[2], and takamasa sakai[2] — [1]Georg-August-Universität Göttingen, Göttingen,Germany — [2]The University of Tokyo, Tokyo, Japan

A theory describing the elastic modulus for percolation networks of Gaussian chains on general lattices such as square and cubic lattices is proposed and its validity is examined with simulation and mechanical experiments on well-defined polymer networks. The theory was developed by generalizing the effective medium approximation (EMA) for Hookian spring network to Gaussian chain networks. From EMA theory, we found that the ratio of the elastic modulus at p, G to that at p = 1, G0, must be equal to G/G0= (p-2/ f)/(1-2/ f) if the position of sites can be determined so as to meet the force balance, where p is the degree of cross-linking reaction. However, the EMA prediction cannot be applicable near its percolation threshold because EMA is a mean field theory. Thus, we combine real-space renormalization and EMA and propose a theory called real-space renormalized EMA, i.e., REMA. The elastic modulus predicted by REMA is in excellent agreement with the results of simulations and experiments of near-ideal diamond lattice gels.

CPP 44.8 Wed 18:15 Poster B2

Tethered Polymers In Shear — •Richard Schwarzl and Roland Netz — Freie Universitaet Berlin, Fachbereich Physik, 14195 Berlin, Germany

We employ Brownian dynamics simulation including hydrodynamic interactions to model the dynamic properties of a polymer under shear flow conditions near a no-slip boundary. Our motivation is the von Willebrand factor, a large glycoprotein in blood. It is a crucial component in regulation of hemostasis. The conformational state of the large multimer determines vWFs ability to bind to other biological components such as collagen or bloodplatelets. Our focus is to build a bridge between single molecule pulling experiments and unfolding of vWF under shear.

CPP 44.9 Wed 18:15 Poster B2

Influence of Spacer Length and Flexibility on the Binding Affinity of Divalent Ligands — •Susanne Liese and Roland R. Netz — Freie Universität Berlin, Fachbereich Physik

We present a quantitative model for the binding of divalent ligand-receptor-systems. We study the influence of the ligand spacer length and flexibility on the overall binding affinity and derive general rules for the optimal ligand design. Therefor, we first compare different polymeric models and determine the probability to simultaneously bind to two neighboring receptor binding pockets. In a second step the binding affinity of divalent ligands in terms of the IC50-value is derived. We find that a divalent ligand has the potential to bind more efficient than its monovalent counterpart only, if the monovalent dissociation constant is lower than a critical value. This critical monovalent dissociation constant depends on the ligand-spacer length and flexibility as well as on the size of the receptor. Regarding the optimal ligand-spacer length and flexibility, we find that the average spacer length should be equal or slightly smaller than the distance between the receptor binding pockets and that the end-to-end spacer length fluctuations should be in the same range as the size of a receptor binding pocket.

CPP 45: Poster: Two Dimensional Functional Materials

Time: Wednesday 18:15–21:00 Location: Poster B2

CPP 45.1 Wed 18:15 Poster B2

Resonant energy-transfer in plasmonic hybrid arrays — •Julian Sindram, Joseph P. S. Fitzgerald, and Matthias Karg — Physical Chemistry I, University of Bayreuth, Bayreuth, Germany

Energy transfer between plasmonic nanoparticles (NPs) and fluorophores drastically alter the spectral response of the involved species and can be harnessed to create plasmonic nanolasers. Such lasers can be nanoscopic sources of coherent light with high potential for many applications in the field of nano-optics. Energy transfer rates depend on various parameters, including the NP material and size, the optical properties of the fluorophore, the distance between NPs and fluorophores and the concentration of fluorophores. In order to achieve a better understanding of energy transfer processes, a screening of numerous parameter combinations is necessary.

We present a new and efficient approach, allowing us to prepare and analyze large parameter sets on a single substrate. A bottom-up preparation procedure is used to fabricate substrate supported silver NP arrays with a spatial gradient of particle sizes. These plasmonic arrays are embedded in a fluorophore host matrix. Position-dependent steady-state and time resolved fluorescence spectroscopy, as well as extinction spectroscopy, are employed to examine energy transfer.

CPP 45.2 Wed 18:15 Poster B2

Fabrication of functional carbon nanomembranes — •Katrin Wunderlich[1], Polina Angelova[2], Armin Gölzhäuser[3], Markus Klapper[1], and Klaus Müllen[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]CNM Technologies GmbH, Bielefeld, Germany — [3]University of Bielefeld, Department of Physics, Bielefeld, Germany

Carbon nanomembranes (CNMs) are important materials for technological applications e.g. filtration of gases or water purification.

Here, we report direct access to functional CNMs starting from small molecules. Three different types of molecules were synthesized: nonfused oligophenyl derivatives with a linear molecular backbone (biphenyl, para-triphenylene), condensed polycyclic precursors (naphthalene, anthracene) and bulky molecules (hexaphenylbenzene, hexaperi-hexabenzocoronene). These aromatics on gold were crosslinked by electron irradiation and pyrolysis. Thus, homogeneous carbon nanomembranes with thicknesses of less than 0.8 nm were obtained.

The thickness, conductivity, chemical functionalization, and appearance of nanopores can be adjusted dependent on the molecule and the resistivity correlates with the thickness of the pyrolysed nanomembrane, with lower resistivity for the thicker sheets.

CPP 45.3 Wed 18:15 Poster B2

Assembly of proteins and oriented purple membrane on functionalized carbon nanomembranes — Natalie Frese[1], •Paul Penner[1], Matthias Schürmann[1], Daniel Rhinow[2], Mark Schnietz[1], Polina Angelova[1], Andrey Turchanin[3], Christian Kaltschmidt[1], Robert Tampé[4], Norbert Hampp[5], and Armin Gölzhäuser[1] — [1]University of Bielefeld — [2]Max Planck Institute of Biophysics, Frankfurt — [3]Friedrich Schiller Universtity Jena — [4]Goethe University, Frankfurt — [5]Philipps University, Marburg

This presentation is about hybrid structures comprising carbon nanomembrane (CNM) as a functional substrate and oriented assembled purple membranes (PMs). CNMs are monomolecular crosslinked layers of aromatic amphiphilic molecules with lateral dimensions of several square centimeters and a thickness of about 1 nm. PM from Halobacterium salinarum is a membrane consisting of bacteriorhodopsin (BR), which is a light-driven proton pump, and lipids. CNM has already been successfully tested as a substrate for electron cryo-microscopy of PM. To realize the oriented assembly of PM patches on CNM, we used a PM mutant, which has histidine (HIS) tags selectively on one side of the membrane and a nitroliotriacetic acid (NTA) terminated NBPT-CNM. The functionalized CNM has also been tested with different HIS-tagged proteins.

CPP 45.4 Wed 18:15 Poster B2

Stimuli-responsive nanosheet thin film sensors — •Pirmin Ganter[1,2], Katalin Szendrei[1,2], Daniel Weber[1,2], and Bettina Lotsch[1,2] — [1]Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart — [2]Department of Chemistry, University of Munich (LMU), Butenandtstraße 5-13, 81377 München

Environmental monitoring as well as breath analysis are of crucial importance in various fields such as health care, agriculture, industrial processes, air quality monitoring and pollution control. Therefore, the development of sensors with a fast response time, high sensitivity and selectivity to specific analytes such as water, ethanol, or other stimuli is highly desirable. Ultrathin sensors can offer several advantages such as cost efficiency or faster response and recovery times. Nanosheet-based sensors inherently feature at least one miniaturized dimension due to their single layer thickness. On this poster we show that phosphatoantimonate nanosheets $H_3Sb_3P_2O_{14}$ can be spin-coated into thin films. These thin films can be used for humidity sensors as well as touchless positioning interfaces due to their extremely high sensitivity, selectivity towards water vapor and fast response time. Furthermore, we present our latest developments on sensing different stimuli such as temperature or trace amounts of water with nanosheet-based thin films.

CPP 45.5 Wed 18:15 Poster B2

Graphene-Enhanced Optical Spectroscopy of Molecular Nano Systems — Bita Rezania[1], •Philipp Lange[1], Nikolai Severin[1], Janina Kneipp[2], and Jürgen P. Rabe[1] — [1]Department of Physics & IRIS Adlershof, Humboldt-Universität zu Berlin — [2]Department of Chemistry, Humboldt-Universität zu Berlin

Graphene enhanced Raman Spectroscopy (GERS) is a newly emerged field. That is, Raman cross sections of molecules located in a close proximity to graphene has been demonstrated to be increased. However, the mechanism of the Raman enhancement in GERS is still not well understood. We investigated GERS on rhodamine 6G (R6G) molecules and we demonstrate a GERS enhancement factor for R6G confined between graphene and mica of about an order of magnitude. To get further insight into the GERS mechanism, we deposited CdTe quantum dots (QD) on top of graphene which covered R6G molecules. The presence of QD on top of graphene results in further enhancement of R6G Raman peaks confined between graphene and mica. The enhancement factor is different for different Raman peaks of R6G. Possible interpretations will be discussed

CPP 45.6 Wed 18:15 Poster B2

2D-sheets covering and replicating single dendronized polymers — •Mohammad Fardin Gholami[1], Simone Dell'Elce[1], Vitalij Scenev[1], Nikolai Severin[1], Baozhong Zhang[2], A. Dieter Schlüter[2], and Jürgen P. Rabe[1] — [1]Institute für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin — [2]Department of Materials, Institute of Polymers, ETH Zurich

Graphene can replicate the topography of a substrate with a precision down to single macromolecules. Here we use this capability and investigate graphene and derivatives thereof for single macromolecules with increasing cross-sections. We deposited dendronized polymers (denpols) onto mica substrates and covered them with graphene oxides (GO), reduced graphene oxides (rGO), and graphenes. The denpols consist of a linear backbone surrounded by a cladding of structurally regular dendritic branches (dendrons), anchored to each repeat unit. The diameter of denpols can be systematically tuned by varying the dendron generation. The height of the molecular imprints in GO agrees well with the height of uncovered molecules. The height of molecular imprints in graphenes is smaller than the height of uncovered molecules with the difference growing with the dendron generation. First results for rGO indicate that the heights of molecular imprints in rGO are in between those for graphene and GO. We attribute the smaller heights under graphenes and rGO to a larger interaction between the sheets and the substrate, effectively squeezing the molecules, implying that the GO-substrate interaction is smaller than that of graphene, allowing for less distortion of the single macromolecules.

CPP 45.7 Wed 18:15 Poster B2

Towards high CO2 capacity: Introduction of amine-containing linkers to HTFG-COF by pre- and post-synthetic methods — •Kerstin Gottschling[1,2], Linus Stegbauer[1,2], and Bettina V. Lotsch[1,2] — [1]Max-Planck-Institut für Festkörperforschung — [2]Ludwig-Maximilians-Universität München

The development of materials that are suitable for the capture, storage and separation of carbon dioxide is an important goal of current research. In this regard, covalent organic frameworks, so-called COFs, stand out as they are light-weight, do not contain problematic elements such as heavy and toxic metals and often show high porosities and gas capacities. The tailoring of HTFG-COF, a hydrazone-based system, towards higher CO2 capacities by the introduction of amine-containing linkers, was investigated. A linker containing terminal tertiary amines was introduced to HTFG-COF by pre- as well as post-synthetic methods. The resulting systems were fully characterized by solid-state NMR spectroscopy, FT-IR, X-ray diffraction and sorption analysis. A significant change of the gas adsorption properties was found and a functionalization grade of 4% for pre- and 8% for post-synthetically modified systems was derived.

CPP 45.8 Wed 18:15 Poster B2

The Structure and Magnetism of Restacked Spin 1/2 honeycomb RuCl3 single layers — •Daniel Weber[1,2], Leslie M. Schoop[1], Viola Duppel[1], Judith M. Lippmann[1,2], Jürgen Nuss[1], and Bettina V. Lotsch[1,2] — [1]Max Planck Institute for Solid State Physics, Heisenbergstr. 1, 70569 Stuttgart — [2]University of Munich, Department of Chemistry, Butenandtstr. 5 - 13, 81377

Spin honeycomb materials have gained substantial interest due to their exotic magnetism. However, in all current materials out-of-plane interactions are interfering with the in-plane order, hence a true 2D magnetic honeycomb system is still of demand. Here, we report the exfoliation of the magnetic semiconductor α-RuCl3 into the first halide monolayers and the magnetic characterization of the spin 1/2 honeycomb arrangement of turbostratically stacked RuCl3 monolayers. The exfoliation is based on a reductive lithiation/hydration approach. After an oxidative treatment, cooperative magnetism due to the spin 1/2 state similar to the bulk can be observed. The oxidized pellets of restacked single layers feature a magnetic transition at $T = 7$ K in the in-plane direction, while the magnetic properties in the out-of-plane direction vastly differ from bulk α-RuCl3. The deliberate introduction of turbostratic disorder to manipulate the spin structure of RuCl3 is of interest for research in frustrated magnetism and complex magnetic order as predicted by the Kitaev-Heisenberg model.

CPP 45.9 Wed 18:15 Poster B2

Chemo- and Bio-Sensor Based on One Dimensional TiO2/SiO2 Photonic Crystals — •Anna-Katharina Hatz[1,2], Ida Pavlichenko[1], and Bettina Lotsch[1,2] — [1]Ludwig-Maximilians-Universität — [2]Max-Planck-Institut für Festkörperforschung

Photonic sensor technologies represent an important milestone in monitoring complex physical, chemical and biological systems. We present a new, biocompatible chemo- and biosensor based on the integration of an one-dimensional (1D) stimuli-responsive photonic crystal (PCs) with an electrophotonic visualisation platform. We demonstrate various modi operandi, including the measurement of the relative pressure of an analyte and the in situ monitoring of adhesive cell cultures, enabled by the modular combination of stimuli-responsive 1D PCs with a LED as light emitter and a photodiode as detector.

CPP 46: Poster: Wetting, Nano- and Microfluidics

Time: Wednesday 18:15–21:00 Location: Poster B2

CPP 46.1 Wed 18:15 Poster B2

Theoretical study of slip effects on a dewetting drop — •Tak Shing Chan[1], Joshua D. McGraw[1,2], Thomas Salez[3], and Martin Brinkmann[1] — [1]Experimental Physics, Saarland University, D-66041, Saarbrücken, Germany — [2]Département de Physique, Ecole Normale Supérieure / PSL Research University, CNRS, 24 rue Lhomond, 75005 Paris, France — [3]PCT Lab, UMR Gulliver 7083, ESPCI ParisTech, PSL Research University, 75005 Paris, France

A recent experimental study on the dewetting of polymer microdroplets have shown that slip plays a dominating role on the shape evolution and the motion of the contact line (Under review). Particularly, a transient bump is observed for relatively small slip lengths, while a bump is avoided for larger values. In this theoretical study, we investigate the dewetting of a drop in a wider regime of parameter space. Using the boundary element method, we solve for the axisymmetric Stokes flow with i) the Navier-slip boundary condition at the solid/liquid boundary, and ii) a time-independent microscopic contact angle at the contact line position. We compute the profile evolution for different slip lengths and equilibrium contact angles. We find that when decreasing the slip length, the characteristic size of the bump first increases, and then decreases. More interestingly, the size of the bump even reaches zero, meaning no bump is observed, if the slip length is small enough. This remarkable result may indicate a crossover to the quasi-static regime when the slip length is very small.

CPP 46.2 Wed 18:15 Poster B2

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

Deformable particles such as capsules, vesicles, and red blood cells assemble at fixed equilibrium positions in a microfluidic channel. This behavior can be used to separate particles with different cell properties. For example, softer cells travel closer to the center than stiffer 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. The steady state of the particles is determined by the lift force profiles, which we determine for different channel aspect ratios.

CPP 46.3 Wed 18:15 Poster B2

Pairs of rigid particles in inertial microfluidics — •Felix Rühle, Christopher Prohm, and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin

We investigate rigid spherical particles in rectangular microchannels under the influence of Poiseuille flow at intermediate Reynolds numbers. It is well known that a single particle shows inertial focussing in this regime [1]. Furthermore, for rectangular channels with sufficiently large aspect ratio only two lateral equilibrium positions exist.

In this contribution we present first results on the behaviour of a particle pair in such a channel thus increasing the complexity of the one-particle system that has already been thoroughly examined [2]. An in-depth understanding of the multi-particle interactions will provide insights into the properties and dynamics of particle chains as well as the formation of so-called microfluidic crystals [3].

The particle pair is placed in the channel with variable axial distance and lateral positions. Inertial migration in the cross section of the channel is quantified by the lift force profile. We determine how it changes due to the presence of a neighboring particle. This helps us to explain the observed passing trajectories, where particles overtake each other, swapping trajectories, and damped oscillations. The latter involve both axial and lateral motion and occur when particles are on opposite sides of the channel centerline.

[1] G. Segré and A. Silberberg, *Nature* **189**, 209 (1961).
[2] C. Prohm and H. Stark, *Lab Chip* **14**, 2115 (2014).
[3] W. Lee et al., *PNAS* **107**, 22413 (2010).

CPP 46.4 Wed 18:15 Poster B2

Super Liquid Repellency — •Frank Schellenberger, Jing Xie, Noemí Encinas, Maxime Paven, Doris Vollmer, and Hans-Jürgen Butt — Max Planck Institute for Polymer Research, Mainz, Germany

The Pandora box of surfaces able to repell liquids is still a hot research topic. These surfaces are able to remove dust (self-cleaning) and can even hinder the growth of microorganism colonies.

Over the past years we have created superhydrophobic coatings (water repellent) where water droplets sit on microscopic pockets of air, which are trapped beneath the liquid drops. We even designed superamphiphobic coatings (i.e. water and oil repellent). One of these types are the so called slippery surfaces, where after infusing a rough/porous structure with a lubricant a deposited drop will slip by tilting the surface by a few degrees. This pressure-stable omniphobicity opens exciting applications for anti-biofouling, anti-icing or anti-frost performances. However, the mechanism how a drop moves on slippery surfaces is still unclear.

In this case, we used Laser Scanning Confocal Microscopy (LSCM) to observe the contact angles and evaluate the dynamics of droplet motion on the microscale.

CPP 46.5 Wed 18:15 Poster B2

Silica stabilized Pickering-emulsions for hydroformylation — •Judith Witte[1], Dmitrij Stehl[1], Regine von Klitzing[1], Tobias Pogrzeba[1], Marcel Schmidt[1], Reinhard Schomäker[1], Lena Hohl[2], Matthias Kraume[2], Tina Skale[3], and Anja Drews[3] — [1]TU-Berlin, Straße des 17. Juni 124, 10623 Berlin — [2]TU-Berlin, Frauenhoferstr. 33-36, 10587 Berlin — [3]HTW Berlin, Wilhelminenhofstr. 75 A, 12459 Berlin

Pickering-emulsions (PEs) are particle stabilized emulsions. PEs can be used for catalytic reactions, for example for the hydroformylation of long chained olefins in a water in oil (w/o-) emulsion. In this study, the water droplets (water phase) which are surrounded by SiO2-nanoparticles as stabilizer, contain [HRh(CO)(TPPTS)3] as homogeneous catalyst. The particle-stabilized water droplets are emulsified in 1-Dodecene (oil phase). After the hydroformylation, the water droplets with the expensive catalyst can be easily separated from the product by membrane filtration and used again for the next reactions. This is a huge advantage in comparison to surfactant stabilized emulsions, which often break during filtration processes. Preliminary experiments showed that an increase in the amount of SiO2-nanoparticles leads to an increase of the product yield (Tridecanal) and decreases the droplet size from 0.02 to 0.005 mm. An addition of surfactant (Triton X-100) at low concentrations (<cmc) increases the product yield as well.

CPP 46.6 Wed 18:15 Poster B2

Contact Line Dynamics and Hydrodynamic Boundary Conditions in Stepped Liquid Films — •Marco Rivetti[1], Thomas Salez[2], Michael Benzaquen[2], Elie Raphaël[2], and Oliver Bäumchen[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), Göttingen, Germany — [2]UMR Gulliver, CNRS and ESPCI ParisTech, PSL University, Paris, France

For flows on the micro- and nanoscale, the physics of the contact line as well as the hydrodynamic boundary condition at a solid surface play a crucial role. In past few years much has been learned about both phenomena from flows that are driven by capillary forces. We here discuss some recent results involving thin liquid films which exhibit slip or no-slip boundary conditions. In the absence of slip, the relaxation of a liquid nanostripe on a smooth, hydrophilic substrate has evidenced the occurrence of, both, stationary and receding contact line regimes [1]. Self-similarity of the liquid profiles in the stationary regime has been proved, and a universal transition between the two regimes has emerged by rescaling with regard to the viscosity, surface tension and film thickness. In the second part we discuss the relaxation of initially perturbed liquid surfaces [2], i.e. stepped liquid films in the absence of contact lines. We find strong evidence that this relaxation process is also sensitive to the slip boundary condition at the solid/liquid interface. Thin film models comprising slip enable a quantification of the slip length of viscous liquids of various molecular properties. [1] Rivetti et al., Soft Matter 11 (2015) [2] McGraw et al., Phys. Rev. Lett. 109, 128303 (2012)

CPP 46.7 Wed 18:15 Poster B2

Fluid invasion in porous media: front morphology, residual saturation, and the Cieplak-Robbins-transition — •Stephan Herminghaus[1], Ralf Seemann[2], Kamaljit Singh[2], Hagen Scholl[2], Marco Di Michiel[3], and Mario Scheel[3] — [1]MPI für Dynamik und Selbstorganisation, Göttingen — [2]Fakultät für Physik, Universität des Saarlandes, Saarbrücken — [3]ESRF, Grenoble

The fluid front morphologies emerging during fluid invasion into random piles of spherical beads are investigated in real time by X-ray micro-tomography and analyzed theoretically. Depending on the wettability of the invaded medium, we observe two distinct displacement regimes exhibiting strongly different liquid front morphologies. These regimes are separated by a pronounced transition, at which the residual saturation of the defending liquid (RSD) changes abruptly by one order of magnitude. We show that the critical contact angle at which this transition takes place can be quantitatively predicted on the basis of a quasi-static consideration of the wetting geometry of the progressing front. Furthermore, we find that the RSD agrees, within experimental scattering, quantitatively with our predictions from analytical theory, without invoking any fitting parameter.

CPP 46.8 Wed 18:15 Poster B2

Particle Confinement by Marangoni Convection in Microchannels — •Michael Orlishausen, Lorenz Butzhammer, and Werner Köhler — Physikalisches Institut, Universität Bayreuth, Universitätsstr. 30 95447 Bayreuth

We have investigated the flow of unary and binary liquids near a liquid-gas interface in a mirochannel device due to Marangoni Convection caused by a gradient in temperature and concentration (in the case of the binary liquids). By using latex microparticles of 1*m diameter we were able to visualize the resulting currents through optical microscopy. Depending on the position of the meniscus in the microchannel and other factors, one or two convection rolls appear. Surprisingly, however, the particles are confined to certain streamlines and regions in the microchannel and characteristic depletion zones form around them. In order to explain the origin of this observation we have performed finite elements simulations to the flow in the microchannel and identified the outermost streamline containing particles as being connected to the minimum distance to the meniscus one of those particles can take up. Additionally, we have investigated the influence of diffusion on particles in such a flow by means of Langevin simulations. The counter-intuitive result is an enhanced particle confinement caused by particle diffusion between different streamlines.

CPP 46.9 Wed 18:15 Poster B2

Onset of motion of a sliding droplet — Simeon Völkel and •Kai Huang — Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany

We investigate experimentally the onset of motion of a water drop on an inclined plane with contact angle hysteresis. The onset of motion is triggered either through increasing the volume of the drop with an inkjet printer head or through tilting the plane with a stepper motor. Based on an analysis of both top view and side view images, we explore the evolution of the drop shape with time in the vicinity of the depinning transition and discuss how different ways to trigger the motion influence the bifurcation scenario of the transition. Finally, we analyze the eccentricity of the drop as a function of bond number that measures the ratio of gravitational forces to surface tension forces and compare our results with numerical simulations.

CPP 46.10 Wed 18:15 Poster B2

Mechanical properties of highly porous super liquid-repellent surfaces — •Maxime Paven, Regina Fuchs, Doris Vollmer, Michael Kappl, and Hans-Jürgen Butt — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

The poor mechanical properties of highly porous materials restrict their utilization for a wide range of applications such as light weighted, insulating or super liquid-repellent coatings. Especially, the design principles of super liquid-repellent surfaces aim at maximizing roughness at the nano or micrometer scale, making them inherently mechanically weak. To find a balance between repellency and stability investigation of the surfaces*s mechanical properties is essential. Here, we use atomic force microscopy, colloidal probe, nanoindentation, and pencil scratching to investigate the mechanical properties of super liquid-repellent surfaces prepared by soot templating. We varied the reaction paramteres, i.e. the thickness of the template-stabilizing silica shell and the sintering temperature to investigate their influence on the wetting and mechanical properties. Sintering at 1000 °C increased the effective elastic modulus of the surface by more than an order of magnitude. Sintering at 1150 °C led to a smoothening of the porous silica network and the effective elastic modulus increased by up to five orders of magnitude. At the same time, however, for droplets of n-hexadecane the roll-off angle increased and the receding contact angle decreased. This emphasizes the delicate balance of stability and repellency for super liquid-repellent surfaces.

CPP 46.11 Wed 18:15 Poster B2

Geometry induced asymmetric contact angles — •Bang-Yan Liu — National Taiwan University, Department of Chemical Engineering, 10617 Taipei, Taiwan — Saarland University, Experimental Physics, D-66041 Saarbrücken, Germany

Triangle post decorated surfaces were studied in this research. Triangular posts were arranged in square lattice and made from PDMS. Asymmetric contact angles were observed, both advancing and receding contact angle in triangle base direction were higher than that in the tip direction. Structures with various triangle sizes and post heights were examined and the three-phase contact line motion was analyzed to study this phenomenon. As water spreading, a strong pinning always happened on the outermost edges of triangular post structure related to droplet center, and with the increase of structure edge presence in three-phase contact line, advancing contact angle raised dramatically. The geometry difference of triangle tip and base resulted in different edge presence of three-phase contact line and caused contact angle asymmetry. However, when the structure height grew, advancing contact angle of both directions increased, and the asymmetry was reduced. On the other hand, de-wetting showed different behavior. Three-phase contact line pinned on the inner edge of structure and one-by-one depinning behavior was observed. Receding contact angle happened when the retreating three-phase contact line depinned from the very last structures to another row of structures. By designing and tuning structure geometry, an easy-produced asymmetry surface can be obtained.

CPP 46.12 Wed 18:15 Poster B2

Wetting Characteristics in Bidisperse Sphere Packings — •Robabeh Moosavi[1], Julie Murison[2], Martin Brinkmann[1,3], and Matthias Schröter[1] — [1]Max-Planck Institute of Dynamics and Self-Organization, Göttingen, Germany — [2]Clariant Produkte GmbH, Competence Center Interface and Formulation Technology, Frankfurt, Germany — [3]Universität des Saarlandes, Saarbrücken, Germany

We report experiments on liquid two-phase flow in bidisperse sphere packings consisting of small and large beads which are either oil wetting or water wetting. Aim of our work is to understand the parameters determining the average wettability of these samples and their residual oil saturation after the packing was invaded by water. The former is studied by measuring the capillary pressure saturation curves [1], the latter by imaging the samples with X-ray tomography. We find that mixed wet samples show a smaller dissipation during a complete drainage/imbibition cycle than when the sample is composed of beads of one type of wetting behavior.

[1] Murison et al., *Phys. Rev. Appl.* **2014**, 2, 034002

CPP 46.13 Wed 18:15 Poster B2

Wettability controls immiscible fluid displacement through local interfacial instabilities — Micheal Jung[1], Martin Brinkmann[1,2], Marta Sanchez de La Lama[2], Thomas Hiller[2], Stephan Herminghaus[2], and •Ralf Seemann[1] — [1]Experimental Physics, Saarland University, Saarbrücken — [2]Max Planck Institute for Dynamics and Self-Organisation

Slow immiscible fluid displacement is studied in a transparent quasi two-dimensional Hele-Shaw cell with cylindrical posts for different wetting conditions of the invading fluid. Employing various combinations of fluids and cell materials allows to cover a range of advancing contact angles θ_a of the invading fluid between 46° and 180° in our experiments. In parallel, we performed numerical simulations of the displacement process employing a particle-based method that accounts for wall wettability in the same arrangements of cylindrical posts as in experiments. A cross-over between capillary fingering at high values of $\theta_a \gtrsim 120°$ and stable interfacial displacement at $\theta_a \lesssim 80°$ is observed in experiments and simulations, and quantified through the front length and the final saturation of the displaced fluid. Analysis of the local displacement processes in experiments and simulations demonstrate that the evolution of the front shape is governed by the local advancing modes for quasi-static interfacial displacement as proposed by Cieplak and Robbins [Phys. Rev. Lett. **60** (1988)]. A comparison of the relative frequency of certain advancing modes reveals a cross-over between cooperative interfacial instabilities for good wetting conditions and non-cooperative instabilities for poor wetting conditions.

CPP 46.14 Wed 18:15 Poster B2

Wetting properties of n-alkane nanostructures — •Diego Diaz[1], Tomas Corrales[2], Maria Retamal[1,3], Marcelo Cisternas[1], Patrick Huber[4], and Ulrich Volkmann[1] — [1]Centro de Investigación en Nanotecnología y Materiales Avanzados, CIEN-UC, Pontificia Universidad Católica de Chile, Santiago, Chile — [2]Instituto de Alta Investigación, Universidad de Tarapacá, Arica, Chile — [3]Facultad de Química, Pontificia Universidad Católica de Chile, Santiago, Chile — [4]Materials Physics, Hamburg U. of Technology, D-21073 Hamburg, Germany

Recently, we have shown that it is possible to modify the surface coverage and morphology of an n-alkane molecular layer over silicon by controlling the withdrawal velocity of the substrate from solution (T.P. Corrales et al., ACS Nano 8, 9954-9963, 2014). As a follow-up work, we study here the wetting properties of silicon surfaces coated with molecular layers of n-alkane as a function of the surface coverage and morphology, using a drop shape analysis procedure. We have found from our measurements that both the coverage and morphology of the underlying nanostructures affects the contact angle of the surface. In particular, stripe-like structures present lower contact angles than dendritic structures that have roughly the same coverage and thickness. All films consist of a single n-alkane molecular layer with a height of around 5 nm. Furthermore, we find differences in the contact angles measured parallel and perpendicular to the withdrawal direction of the substrate from solution.

CPP 47: Poster: Interfaces and Thin Films

Time: Wednesday 18:15–21:00 Location: Poster B2

CPP 47.1 Wed 18:15 Poster B2

Metal ions at metal/polymer interfaces — •Maria Sonnenberg[1], René Gustus[1], Wolfgang Maus-Friedrichs[1], Herbert Scheerer[2], Juan Pablo Vega Triana[2], Sascha Sedelmeier[3], and Jürgen Wieser[3] — [1]Clausthaler Zentrum für Materialtechnik, Agricolastraße 2, 38678 Clausthal-Zellerfeld, Germany — [2]Zentrum für Konstruktionswerkstoffe, Grafenstraße 2, 64382 Darmstadt, Germany — [3]Frauenhofer LBF, Schlossgartenstraße 6, 64289 Darmstadt, Germany

Understanding the interaction between thin polymer films and metal surfaces is necessary for the plastics processing industry. During the processing of plastic, polymer is melted in the extruder unit. Often thin polymer layers are formed on the surface of the extruder, which leads to peeling off of partly solidified polymer into the melt. These polymer particles will not melt again and generate weak points within the product. Basic understanding of these mechanisms is important in order to avoid steel/polymer interaction. For this purpose thin layers of polycarbonate were prepared by bottom up procedures on different metal substrates and heated up to 280°C. The interfaces were examined by electron spectroscopic (XPS, AES) and microscopic (SEM, AFM) techniques. Experiments show that the diffusion of iron ions in the polymer melt occurs. Same characteristics could not be found for thin polymer layers on chromium substrate. Further experimental results and a mechanism of iron diffusion in thin polymer layers will be shown.

CPP 47.2 Wed 18:15 Poster B2

Mesostructured ZnO scattering layers for OLED applications — •Lorenz Biessmann[1], Christoph J. Schaffer[1], Johannes Schlipf[1], Volker Körstgens[1], Sigrid Bernstorff[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Elettra Sincrotrone Trieste, 34012 Basovizza, Italy

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

CPP 47.3 Wed 18:15 Poster B2

Molecular dynamics of itraconazole confined in thin supported layers — •Emmanuel Urandu Mapesa[1], Magdalena Tarnacka[2], Ewa Kamińska[2], Wilhem Kossack[1], Martin Tress[1], Wycliffe Kipnusu[1], Kamil Kamiński[2], and Friedrich Kremer[1] — [1]Institute for Experimental Physics I, University of Leipzig, Linnestr. 5, 04103, Leipzig, Germany. — [2]Institute of Physics, University of Silesia, ul. Uniwersytecka 4, 40-007 Katowice, Poland.

Broadband Dielectric Spectroscopy (BDS) is used to study the molecular dynamics of thin layers of itraconazole - an active pharmaceutics ingredient with rod-like structure and whose Differential Scanning Calorimetry (DSC) scans reveal liquid crystalline-like phase transitions. It is found that (i) the structural relaxation process remains bulk like, within the limits of experimental accuracy, in its mean relaxation rate, while (ii) its shape is governed by two competing events: interfacial interactions, and crystalline ordering. Additionally, (iii) the dynamics of the delta-relaxation - assigned to the flip-flop rotation of the molecule about its short axis - deviates from bulk behaviour as the glass transition is approached for the confined material. These observations are rationalized within the framework of molecular dynamics as currently understood.

CPP 47.4 Wed 18:15 Poster B2

Artificial nanostructuring of thin conjugated polymer films — •Ali Özkü, Franziska Löhrer, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Conjugated polymer films have received great attention due to many applications in organic electronics, as for example organic solar cells. In particular, novel low band gap polymers have shown to give rise to high power conversion efficiencies. An artificial nanostructuring of the polymer films can add an additional benefit with regard to applications, as for example the photon management can be tailored. In the present work, we combine low band gap polymers with an artificial nanostructuring of the polymer film by soft embossing methods. The optical properties of nanostructured thin films are investigated with UV/Vis and photoluminescence measurements. Morphological studies include optical microscopy, AFM and X-ray diffraction methods. From a combination of these findings, we aim on establishing a structure-function relationship.

CPP 47.5 Wed 18:15 Poster B2

Degradation in printed polymer:fullerene thin films for organic photovoltaics — •Jan Richard Stockhausen, Christoph J. Schaffer, and Peter Müller-Buschbaum — TU München, Physik-Department, James Franck-Str. 1, 85748 Garching

In comparison to conventional silicon solar cells, organic solar cells offer several advantages, such as ease of production in large-scale and high versatility. Nevertheless, their lifetime needs to be prolonged, so that a profitable application on a large-scale becomes feasible. Therefore a detailed understanding of all degradation mechanisms is necessary. In the present investigation we address UV and visible light induced aging of P3HT:PCBM active layers. Instead of spin coating, positive shim mask guided slot dye coating is used for film fabrication as large-scale production will most probably rely on printing techniques. Therefore several irradiation chambers are built to expose the films to radiation of different wavelengths. Changes in the films due to accelerated aging are investigated by means of AFM, X-ray reflectivity and UV/Visible light spectroscopy.

CPP 47.6 Wed 18:15 Poster B2

Thin P3HT:PCBM films with embedded magnetic nanoparticles — •Florian Dreher, Daniel Moseguí González, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Among the different photoactive systems studied in organic solar cells, the combination of P3HT:PCBM has been most prominent due to easy chemical synthesis and, thus, commercial availability. In order to further increase the device performance, doping with magnetic nanoparticles had shown interesting behavior as the device efficiency can be increase upon nanoparticle addition.[1] In the present study we focus on thin P3HT:PCBM films and investigate the impact of different concentrations of magnetic nanoparticles under various processing conditions. The film morphology is probed with SEM, AFM and scattering techniques. UVvis spectroscopy and photoluminesces measurements complement these morphology studies. In combination with device characterization we gain a structure-function relationship for these thin hybrid films.

[1] Moseguí González et al.; Adv. Energy Mater. 5, 1401770 (2015)

CPP 47.7 Wed 18:15 Poster B2

Athermal Azobenzene-Based Nanoimprint Lithography — •Christoph Meichner[1], Lothar Kador[1], Christian Probst[2], Klaus Kreger[2], Christian Neuber[2], and Hans-Werner Schmidt[2] — [1]University of Bayreuth, Institute of Physics and Bayreuth Institute of Macromolecular Research (BIMF), 95440 Bayreuth, Germany — [2]University of Bayreuth, Macromolecular Chemistry I and Bayreuth Institute of Macromolecular Research (BIMF), 95440 Bayreuth, Germany

We present athermal micro- and nanoimprint lithography as a new method, using a photoresponsive azobenzene-based molecular glass as resist material. Patterning with this approach is based on athermal photofluidization, i.e., a photoinduced decrease in viscosity far below the T_g of the material, enabling mass transport at ambient conditions during light irradiation. In contrast to common imprint techniques, no crosslinking or curing steps are involved. The method is capable of patterning nanostructures without being limited to periodic structures or the dimension of the light wavelength. Our investigation includes the presentation of the basic principle and the characterization of influencing factors such as wavelength and fluence of the light and film thickness. Micrometer-sized structures of 100 nm height can be imprinted within approximately 200 s. The feasibility of imprinting very precise structure replica down to 100 nm line width is demonstrated. It is found that decreasing structure sizes lead to increased filling times.

CPP 47.8 Wed 18:15 Poster B2

The formation of micro-porous structure in different polystyrene-based polymers — •Farid Farajollahi, Masoud Amirkhani, and Othmar Marti — Institute of Experimental Physics, University of Ulm, 89069 Ulm, Germany

Breath figure technique is a self-assembly method to produce porous structure on the surface of polymers under the humid condition. The water condensation creates several small droplets, which can be used as templates to make the porous structure after drying the polymer. Generally, hydrophobic polymers such as polystyrene cannot form the close-packed porous pattern in most cases. Here, we developed a new strategy to employ several polystyrene-based polymers to make porous honeycomb structures. The proper concentration of methanol in the polymer solution can improve the stability of water droplets during porous pattern formation. The effect of polymer molecular weight and monocarboxy end terminated group in the morphology of the patterns are investigated by the scanning electron microscopy. In addition, Voronoi diagram is utilized to compare the regularity of the different patterns. Finally, the viscosity measurement is performed to find the relation between pattern morphologies and the initial viscosity of the solutions.

CPP 47.9 Wed 18:15 Poster B2

Towards 3d single particle orbit tracking in multiblock copolymer membranes — •Daniel Zalami[1], Oliver Grimm[2], Felix H. Schacher[2], Jürgen Köhler[1], and Uwe Gerken[1] — [1]Experimental Physics IV and Bayreuth Institute of Macromolecular Research (BIMF), University of Bayreuth, Germany — [2]Institute for Organic Chemistry and Macromolecular Chemistry (IOMC) and Jena Centre of Soft Matter (JCSM), Friedich-Schiller University Jena

The method of *single particle orbit tracking* (SPOT) permits to record the trajectories of fluorescent particles in three dimensions for long observation times (up to tens of minutes) [1,2]. This versatile technique can be applied in the field of life sciences as well as in the materials chemistry. We want to investigate the diffusion behavior of tracer particles within different block copolymer membranes with a stimuli-responsive block covering the pore surface [2]. Our aim is to adress changes in the trans-membrane and intra-membrane transport parameters as a function of the particle properties or variations of the environmental conditions.

[1] V. Levi, Q. Ruan, E. Gratton, Biophys. J., 88, 2919-2928 (2005)
[2] D. Ernst. S. Hain, J. Köhler, J. Opt. Soc. Am. A, 29, 1277-1287 (2012)
[3] F. Schacher, M. Ulbricht, A. H. E. Müller, Adv. Funct. Mater. 19, 1040-1045 (2009)

CPP 47.10 Wed 18:15 Poster B2

Force response of actively deformed polymer microdroplets and -films: dependence on the solid/liquid boundary condition — •Jonas R. Heppe[1,2], Joshua D. McGraw[2,3], Roland Bennewitz[1], and Karin Jacobs[2] — [1]INM - Leibniz Institute for New Materials, D-66123 Saarbrücken — [2]Saarland University, Experimental Physics, D-66041 Saarbrücken — [3]Ecole Normale Supérieure, Département de Physique, F-75005, Paris

In fluid dynamics, the solid/liquid boundary condition can play a major role in the flow behavior of a liquid. For example, in the dewetting of identical polymer films on weak slip or strong slip substrates, large qualitative and quantitative differences are observed. Therefore, when applying an external load to a liquid resting on such substrates, the measured reaction forces and the ensuing flow should also depend on the boundary condition. We present atomic force microscopy measurements in which the reaction force of a cantilever is measured as the tip pierces micron-sized droplets and films of polymeric liquid. These indentations are done on substrates with tuned slip. Accessing the size, depth and rate dependence of the resulting force distance curves, we show an influence of the slip condition on the dissipated energy and adhesion.

CPP 47.11 Wed 18:15 Poster B2

Morphological changes in diblock copolymer thin films in solvent vapor mixtures — •Florian Jung[1], Anatoly V. Berezkin[1], Detlef-M. Smilgies[2], Dorthe Posselt[3], and Christine M. Papadakis[1] — [1]Technische Universität München, Physik-Department, Garching, Germany — [2]Cornell University, CHESS Wilson Lab, Ithaca, NY, U.S.A. — [3]Roskilde University, Department of Science, Systems and Models, Denmark

Block copolymers self-assemble and form various morphologies. Thin films have been proposed for nanolithography. Solvent vapor annealing increases the mobility of the polymers, which can lead to an improved long-range order. In the present work, solvent vapor annealing was carried out using a mixture of vapors of two different solvents that both are selective for one block. Thin films from a cylinder-forming polystyrene-block-poly(dimethylsiloxane) diblock copolymer were prepared on Si wafers. The morphological changes were investigated by in-situ, real-time grazing-incidence small-angle X-ray scattering, varying the degree of swelling of the film, the mixing ratio of the two solvent vapors and temperature. Varying the solvent vapor composition systematically reveals a path dependence of the resulting morphology.

CPP 47.12 Wed 18:15 Poster B2

Diffusion measurements on organic coatings with cantilever beam deflection method — •Franziska Rosensteiner and Sabine Hild — Johannes Kepler University, Linz, Austria

Organic coatings are used to protect steel bands from corrosion which is important i.e. in the building industry. To enhance the barrier properties of organic coatings to achieve better quality of the product improved knowledge about the influence of glass transition temperature Tg and water diffusion properties is necessary. A climatic chamber equipped with a cantilever beam deflection set-up has been developed and built which enables to control and regulate temperature and humidity simultaneously. As samples coated steel band cut into cantilever (4.5 mm x 0.5 mm) are used which are fixed in a special sample holder. Due to the different expansion coefficient of steel and the polymer coating used varying temperatures and humidity lead to characteristic bending of the cantilever due to internal stresses. The cantilever bending is monitored using an optical deflection sensor. From the resulting deflection curves characteristic values such as Tg, as well as the water diffusion constant can be determined. Besides, the way how water diffuses through the coating may explain details about its barrier properties. Therefore, in addition to the cantilever beam deflection measurements the passway of the water adsorbed from the gasous and liquid phase inside the coating is analysed with confocal Raman microcopy.

CPP 47.13 Wed 18:15 Poster B2

Dielectric properties of water in carbon nanotubes — •Philip Loche, Alexander Schlaich, and Roland R. Netz — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14 14195 Berlin

Dielectric properties of confined fluids are important for understanding elementary processes in nanofluids and nanochemistry. Especially cylindrical geometries are of great interest because their applications cover transport through membrane proteins, desalination via nanopores, or transport processes in carbon nanotubes (CNT).

We use Molecular Dynamics Simulations to investigate the dielectric properties of SPC/E water confined in CNTs as model for cylindrical cavities. Comparing various radii and lengths, our results show a high anistropy. Additionally, we perform a finite size scaling of the influence of the nanotube length and compare to the expectation of simple arguments of statistical mechanics.

CPP 47.14 Wed 18:15 Poster B2

Adsorption of acid-hydrolysed soy protein on hydrophobic surfaces studied with x-ray reflectivity — Paul Salmen[1], Julia Nase[1], •Steffen Bieder[1], Patrick Degen[2], Yury Forov[1], Lena Heuchel[1], Florian Wirkert[1], Michael Paulus[1], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Physikalische Chemie 2, Technische Universität Dortmund, 44221 Dortmund, Germany

The adsorption of denaturized or fragmented proteins is important for many applications in industry and biology. We investigated the adsorption of soy sauce and acid hydrolyzed soy protein on hydrophobic, octadecyltrichlorosilane coated silicon wafers and at the air/water interface with x-ray reflectivity. For acid hydrolyzed soy protein, a concentration dependent adsorption is visible at both interfaces. The adsorbed layers have a thickness in the nm range and change the surface properties, like wettability and contact angle, strongly. Also, we were able to show that the amount of adsorbed protein fragments is correlated with the hydrophobicity of the interfaces.

CPP 47.15 Wed 18:15 Poster B2

Ausrichtung von Farbstoffmolekülen in vertsreckten Polypropylenfilmen — •Martin Schindler, Stefan Krause, Christian von Borczyskowski und Robert Magerle — Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Germany

Die Fluoreszenzpolarisation von Farbstoffmolekülen ist eine empfindliche Sonde für die Orientierung der Farbstoffmoleküle in einem Polymerfilm. Wir untersuchten mittels Fluoreszenzpolarisationsmikroskopie das Reorientierungs- und Relaxationsverhalten funktionalisierter Perilenbisimidmolekülen in Polypropylenfilmen als Funktion der Dehnung des Polymerfilms, der mit einem Mikrozugversuch uniaxial verstreckt wird. Aufgrund der Sphärolithmorpholigie des teilkristallinen Polypropylens erwarten wir ein räumlich heterogenes Verhalten: An den amorphen Grenzen zwischen den Sphärolithen erfolgt eine große lokale Dehnung. Die in diesen Bereichen eingebetteten PBI-Moleküle sollten eine größere Ausrichtung entlang der Dehnungsrichtung aufweisen als in Sphärolithen eingebaute PBI-Moleküle.

CPP 47.16 Wed 18:15 Poster B2

Human apolipoprotein A1 at water - solid and water - gas interfaces — •Susanne Dogan[1], Michael Paulus[1], Irena Kiesel[2], and Paul Salmen[1] — [1]Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund, Germany — [2]Institut Laue-Langevin, 71 avenue des Martyrs, 38000 Grenoble, France

The adsorption behaviour of human apolipoprotein A1 (Apo A1) at hydrophilic and hydrophobic interfaces was studied by means of X-ray reflectometry. Apo A1 is a transport protein and part of the high density protein (HDL) which is responsible for the transport of lipids, mainly cholesterol from the cell membranes to the liver. Due to its anisotropic surface, Apo A1 is able to interact with surfaces or interfaces via different interaction mechanisms including the hydrophobic and electrostatic interaction. pH dependent measurements at the solid - water interface between silicon dioxide and aqueous protein solution show that in a small pH range between pH 3 and pH 5 adsorption is increased due to electrostatic attraction. Here the native shape of the protein is altered, in order to maximize the contact with the interface. In contrast, the strong hydrophobic interaction between the protein and the liquid-gas interface yields the denaturation of the protein.

CPP 47.17 Wed 18:15 Poster B2

Oxidation behavior of $Si_xH_yN_z$ films prepared via plasma-enhanced chemical vapor deposition — •Sebastian Dahle[1,2], Jan-Stefan Peters[1,2], and Wolfgang Maus-Friedrichs[1,2] — [1]Clausthaler Zentrum für Materialtechnik, Technische Universität Clausthal, Leibnizstr. 9, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Energieforschung und Physikalische Technologien, Technische Universität Clausthal, Leibnizstr. 4, D-38678 Clausthal-Zellerfeld, Germany

Abstract: The deposition of silicon-containing films is possible in a very simple manner via plasma-enhanced chemical vapor deposition (PECVD). A dielectric barrier discharge (DBD) plasma was used to prepare $Si_xH_yN_z$ films from 1.5% monosilane (SiH_4) diluted in nitrogen. These films were easily transformed into stoichiometric silicon dioxide (SiO_2) by a second DBD treatment in either oxygen or air. Further, the $Si_xH_yN_z$ films were sensitive to atmospheric air even without plasma excitation, although a simple exposure to air was not able to completely transform it into stoichiometric SiO_2. However, the morphology of the resulting silicon oxide (SiO_x) films severely depended on the pressure and the gas used to oxidize the PECVD primer films.

CPP 47.18 Wed 18:15 Poster B2

Molecular Structure of Photo-switchable Azo Dye/Surfactant Mixtures at Air-Water Interfaces — •Saskia Streubel, Felix Schulze-Zachau, and Björn Braunschweig — Friedrich-Alexander University Erlangen-Nürnberg (FAU), Institute of Particle Technology (LFG), Erlangen, Germany

Adsorption and molecular structure of disodium 6-hydroxy-5-[(4-sulfophenyl)azo]-2-naphthalenesulfonate (Sunset Yellow) dye mixtures with cetyltrimethylammonium bromide (CTAB) surfactants was studied at air/water interfaces using tensiometry, ellipsometry and vibrational sum-frequency generation (SFG). In addition to effects of the mixing ratio on interfacial adsorption, we have investigated in detail the influence of light-induced isomerization of Sunset Yellow dye and its complexes with CTA^- ions on the molecular structure at air/water interface. Here, different isomers were generated by irradiating the samples with UV light which leads to less-hydrophobic cis-isomers, while backward transformation to trans-isomers could be achieved by blue light. In addition to information on interfacial composition, conformation and charging state that was gained by applying SFG spectroscopy and ellipsometry, we have investigated the properties of macroscopic foam as a function of mixing ratio and UV light exposure and deduce structure-property relations from the molecular to the macroscopic level.

CPP 47.19 Wed 18:15 Poster B2

Dose and energy dependent chemical modification of ultrathin polymer films as studied by STXM — Markus Meyer[1], Andreas Späth[1], Benjamin Watts[2], and •Rainer H. Fink[1] — [1]FAU Erlangen-Nürnberg, PC II, Erlangen, Germany — [2]SwissLight Source, Paul Scherrer Institut, Villigen, Switzerland

Organic molecules are very sensitive to intense UV or XUV irradiation which may induce severe chemical modifications. We have employed scanning transmission x-ray microspectroscopy to investigate the influences of photon energy, photon flux and illumination sequence (for different energies) to explore effects like mass loss (due to bond rupture) or chemical changes. In our studies we investigate ultrathin free-standing films of poly-methyle methacrylate (PMMA), polylactic acid (PLA) and polystyrene (PS). The aims specifically focus on the impact of secondary electrons after near-threshold, on-resonance and high-energy irradiation (30 or 100 eV above resonance). It is found that the absorbed dose as a common criterion for induced damage does not necessarily correlate with the observed chemical damage. We conclude a destabilization of respective bonds due to resonant excitation, thus resulting in a higher probability of subsequent bond cleavage and simultaneous formation of new species. Kinetic studies comparing resonant and non-resonant excitations and degradation processes of the chemical structure complete the studies. Profound understanding of mechanisms in the interplay of irradiation with soft matter, allow to prevent and avoid sample degradation and in particular cases take advantage of the introduced, controlled chemical modification.

CPP 47.20 Wed 18:15 Poster B2

Comparison of the Swelling behavior of thin cross-and non-crosslinked ethylene glycol based polymer film — •Jessica Hübner, Dikran Kesal, Stefan Wellert, and Regine von Klitzing — Stranski Laboratorium f. Physikalische und Theoretische Chemie, TU Berlin, Str. d. 17. Juni 124, Berlin 10623, Germany

Two intensively studied classes of coatings are polymer brushes and layers of microgel particles at planar solid surfaces. Brushes are polymers, tethered at one end to the substrate while microgels are colloidal particles with an inner polymer network structure based on chemical cross-linking. Here, we compare the properties of ethylene glycol based brushes and microgel particles at silicon surfaces in terms of their swelling/deswelling behavior and volume phase transition temperature depending on comonomer content and synthesis conditions. For both systems the monomer was 2-(2-Methoxy-ethoxy)ethyl methacrylate and the comonomer Poly(ethylene glycol)methyl ether methacrylate. In both architectures, the volume phase transition temperature can be tailored by changing the amount of comonomer. Beside ellipsometry also AFM measurements under ambient conditions and in the water swollen state were used to characterize the brushes and micogels.

CPP 48: Focus: The Physics of Water Interactions with Biological Matter (joint session BP/CPP, organized by CPP)

Organizers: Emanuel Schneck (MPIKG Potsdam), Regine von Klitzing (TU Berlin), Tristan Bereau (MPIP Mainz)

The role of water in biological systems is not simply to act as a solute for biomolecules. Water mediates the interaction between biological interfaces and has to be considered an integral component of biomolecular assemblies. These interactions can alter the properties of both water and the biomolecules in significant ways. Recent methodological progress in experimental techniques and computer simulations provides us with improved tools to gain insight into the relevant physics, from quantum-chemical details of individual molecules, to collective behavior at interfaces, to hydration-dependent structures of biomaterials. The purpose of this Focus Session is to bring scientists from various disciplines to search for solutions to integrate hydration phenomena on different length scales.

Time: Thursday 9:30–12:45 Location: H37

Invited Talk CPP 48.1 Thu 9:30 H37

It is water what matters: THz absorption spectroscopy as a new tool to study solvation dynamics — •Martina Havenith — Physikalische Chemie II, Ruhr-Universität Bochum, Bochum, Germany

Terahertz (THz) absorption spectroscopy is a powerful tool to study (bio)molecular hydration. Experimental advances in the development of new THz sources had to go hand in hand with the development of new theoretical concepts which are able to describe the underlying solute-induced sub-picosecond dynamics of the hydration shell.

Recent results show the significance of hydrogen bond dynamics for molecular recognition. We find a gradient of water motion toward functional sites of proteins, the so-called "hydration funnel", which is found to be essential for biomolecular function.

Transient THz spectroscopy can be used to record snapshots of the low frequency spectrum of a solvated proteins during protein folding, thus capturing changes during hydrophobic collapse in real time during biological function. Within the talk I will present examples of low frequency spectra of hydration water around solutes which can be correlated to changes in entropy.

V. Conti Nibali, M. Havenith New insights into the role of water in biological function: Studying solvated biomolecules using terahertz absorption spectroscopy in conjunction with molecular dynamics simulations J. Am. Chem. Soc. 136(37), 12800-12807 (2014)

CPP 48.2 Thu 10:00 H37

The Effect of Zwitterionic Ectoine on Local Water Dynamics — •Johannes Zeman and Jens Smiatek — Institute for Computational Physics, University of Stuttgart, Germany

Ectoine is known to have a stabilizing effect on proteins in aqueous solution. In order to investigate the plausibility of a suggested indirect mechanism [1], its effect on the local water dynamics at low molar concentrations has been examined by means of Molecular Dynamics simulations. The simulation data has been analyzed in terms of diffusion coefficients, hydrogen bond life times and angular distributions, power spectra, as well as dielectric spectra.

The observed influence of zwitterionic ectoine on water dynamics indicate a pronounced structural strengthening and therefore support the hypothesis of an indirect stabilization mechanism.

For comparison, similar simulations and analyses have been carried out with urea in aqueous solution, as urea is known to have a denaturing effect on proteins. As expected [2], the influence of urea on the local water dynamics is comparatively small.

[1] M. B. Hahn et al., The Influence of the Compatible Solute Ectoine on the Local Water Structure: Implications for the Binding of the Protein G5P to DNA, J. Phys. Chem. B (Nov 10, 2015) [Epub ahead of print]

[2] D. Bandyopadhyay et al., Molecular Dynamics Simulation of Aqueous Urea Solution: Is Urea a Structure Breaker?, J. Phys. Chem. B, 118 (40), pp 11757–11768 (2014)

Invited Talk CPP 48.3 Thu 10:15 H37

Dielectric and diffusional aspects of hydration water — •Roland Netz and Matej Kanduc — Physics Department, FU Berlin, Germany

The molecular layer of water molecules on surfaces is important for the properties of neutral and charged solutes and surfaces. We study how hydration and dielectric properties of interfacial water layers can be used to explain diverse phenomena such as the hydration repulsion between polar surfaces, dielectric spectra of salt solutions, and conformational transitions of polymers.

CPP 48.4 Thu 10:45 H37

Salt Induced Hydrophobic Polymer Collapse Theoretical Model vs. Simulation — •Jan Heyda[1] and Joachim Dzubiella[2,3] — [1]Department of Physical Chemistry, University of Chemistry and Technology, Prague, Czech Republic — [2]Soft Matter and Functional Materials, Helmholtz- Zentrum Berlin, Hahn-Meitner Platz 1, 14109 Berlin, Germany — [3]Department of Physics, Humboldt-University Berlin, Newtonstr. 15, 12489 Berlin, Germany

Smart materials are perspective due to their versatility. An soft-matter example are thermoresponsive polymers, which undergo volume transition, when crossing the lower critical solution temperature (LCST). Near the LCST, they become sensitive to other stimuli, such as salt type and concentration (dx.doi.org/10.1021/ja0546424).

In this contribution, we employed a hydrophobic polymer model (dx.doi.org/10.1073/pnas.0605139104), which possesses 2-state behavior, to study ion-specific effects. We performed replica-exchange molecular dynamics simulations and analyzed the data thermodynamically as well as in terms of Kirkwood-Buff theory, i.e., the preferential binding of salt over water to the polymer was determined.

We have found that the effect on LCST change of salts excluded from hydrophobic interfaces, such as KF and NaCl is strikingly different from attracted salts, such as NaI or GndCl. The surface area based model performs well for the first, but fail for the second group of salts.

To interpret the effect of 'binding' salts, we have employed recently proposed bridging mechanism (dx.doi.org/10.1021/ma302320y) and chain configuration entropy approach (dx.doi.org/10.1039/c4cp05314a).

15 min. break

Invited Talk CPP 48.5 Thu 11:15 H37

Neutron scattering clarifies the behaviour of water in cells — •Giuseppe Zaccai — Institut Laue Langevin, Grenoble, France

Its essential role in biological structure and function is so well established that the search of extra-terrestrial Life is guided by a search of liquid water. Yet the H-bonding properties of water and their interactions with biological molecules are still not fully understood. Because of the strong H/D isotope effect in neutron scattering, neutron diffraction and neutron spectroscopy are particularly powerful experimental methods for the study of water in biology. Neutrons contributed important data to clarify the state of water in cells, following controversial reports on its dynamic state, which, by sustaining that in cell conditions are significantly different, put in question the relevance of in vitro studies. The atomic scale dynamics of intracellular water has been measured in vivo in mesophile and extreme halophile organisms. The results clearly show that intracellular water, other than in hydration interactions with macromolecules and membranes, flows as freely as bulk water, with similar effects on functional molecular dynamics as observed in vitro. Neutrons also characterised the state of water in the intracellular solvent of halotolerant bacteria, which contains molar concentrations of the compatible solute ectoine. All these observations underline the biological requirement of maintaining, within the physiological environment, the remarkable H-bonding properties of liquid water.

CPP 48.6 Thu 11:45 H37

Explicitly implicit solutions: Cavity optimization on the cheap — •David Egger, Christoph Scheurer, Karsten Reuter, and Harald Oberhofer — Technische Universität München, Garching, Germany

In recent years the importance of the solvent response in catalytic, bio- and photochemical processes has become more and more apparent. Yet, in ab-initio computer simulations treating the solvent effect in an efficient but accurate manner is still a major challenge. Unfortunately, an explicit inclusion of solvent molecules significantly increases the associated computational costs. Therefore, continuum solvation models which treat the solute-solvent interaction implicitly through their dielectric permittivities, are often the method of choice. The transitions between these permittivities define a dielectric 'cavity' that is generally defined over free parameters.

In our contribution, we study the validity of such an approach by comparing the implicit potential response to that of explicit classical MD simulations. We reverse engineer an optimal cavity by minimizing the differences between explicit and implicit spatially resolved electrostatic reaction potential of the solvent. To this end we also investigate a number of different models of the permittivity transition function and cavity. Finally, we present optimization results for ions and small molecules in water.

Invited Talk CPP 48.7 Thu 12:00 H37

Controlling Water Evaporation: self-assembly at air/liquid interfaces — •Emma Sparr[1] and Kevin Roger[2] — [1]Physical chemistry, Lund University, Sweden — [2]Université de Toulouse, France

Land-living organisms face the challenge that the ambient air is much drier than what is found in a living cell. One strategy to counter this drying-out threat is through lipid-protein barrier membranes, like the human skin. One important property of the skin is that the evaporation rate across skin is nearly independent of the air humidity, which implies that skin is a responding membrane and its permeability depends on its boundary conditions.

Using aqueous solutions of amphiphilic molecules, we show that the response can be explained by changes in self-assembly structures in the water gradient across the interfacial layer. We have designed an experimental device coupled to a variety of characterization techniques (X-ray scattering, polarized & IR microscopy) to study the non-equilibrium time evolution at an air- liquid interface. Using this device we demonstrate for two model systems how multilayer interfacial structures are formed, and how these structures influence the water transport. We show that a dry phase with low water permeability forms at the air/liquid interface and adapts its thickness to counter changes in the air humidity. This responsive shield is a universal feature of systems for which the structure/permeability changes with the water content. Our findings can unveil mechanism of responding membrane in biological systems, for example, the skin, and it can lead to new possibilities to design robust and homogeneous coatings of amphiphilic molecules.

CPP 48.8 Thu 12:30 H37

Anomalous and anisotropic diffusion of hydration water in fluid lipid membranes — •Felix Roosen-Runge[1], Laura Toppozini[2], and Maikel Rheinstädter[2] — [1]Institut Laue-Langevin, Grenoble, France — [2]McMaster University, Hamilton, Ontario, Canada

Water diffusion in heterogeneous environments is a relevant and frequently studied phenomenon in experiment, simulation and theory. We report on water diffusion between phospholipid membranes using incoherent quasi-elastic neutron scattering (QENS) and computer simulations [1]. The combination of a well-aligned stack of DMPC membranes with the large, 2-dimensional detectors available at the neutron spectrometer Let (ISIS, UK) allows for simultaneous access to water motions lateral and perpendicular to the membranes. The resulting 2-dimensional maps of relaxation time, τ, and stretching exponent, β, evidence anomalous (sub-diffusive) and anisotropic diffusion of membrane hydration water varying on nanometer distances. By combining molecular dynamics and coarse-grained Brownian dynamics simulations, the overall behavior is reproduced, and the apparent features can be linked back to an intrinsic sub-diffusivity of water at picosecond time scales, and the anisotropy of confinement and local dynamical environments.

[1] Toppozini et al. Soft Matter 11 (2015) 8354

CPP 49: Organic Electronics and Photovoltaics II (joint session CPP/DS/HL/O, organized by CPP)

Time: Thursday 9:30–12:45 Location: H40

Invited Talk CPP 49.1 Thu 9:30 H40

Patterned organic ferroelectric memory diodes by solution micromolding — •Paul Blom, Thomas Lenz, Simon Benneckendorf, Kamal Asadi, and Dago de Leeuw — Max Planck Institute for Polymer Research, Ackermannweg 10, Mainz, Germany, D-55128

Ferroelectric polymers are promising candidates for memory technology, since they provide two bistable non-volatile polarization states corresponding to a Boolean 1 and 0, which can repeatedly be switched by an external field. The most widely investigated organic ferroelectric is the copolymer of poly(vinylidene fluoride) and trifluoroethylene (P(VDF-TrFE)). However, implementation of ferroelectric capacitors into integrated circuits is hampered by the read-out of the information being destructive. This problem can be overcome by using phase separated blends of P(VDF-TrFE) with a semiconducting polymer. The bistable polarization state of the P(VDF-TrFE) yields the binary information that can be read-out non-destructively by the current through the semiconducting columns. Phase separation however is a random process that yields a spatially undefined microstructure. Here we use solution micromolding to obtain a linear grating of P(VDF-TrFE). he space in between the lines is backfilled with a semiconducting polymer, resulting in a binary array between two electrodes. The resulting ferroelectric diode can be programmed reversibly in a low resistive on-state and high resistive off-state. When the bias is turned off, the information is retained. The performance can be optimized by down scaling the lateral dimensions of the binary array.

CPP 49.2 Thu 10:00 H40

A new Figure of Merit for Organic Solar Cells with Transport-limited Photocurrents — •Dieter Neher[1], Juliane Kniepert[1], Arik Elimelech[1], and L. Jan Anton Koster[2] — [1]University of Potsdam, Potsdam, Germany — [2]Zernike Institute for Advanced Materials, Groningen, The Netherlands

Organic semiconductors exhibit superior absorption properties but suffer from low mobilities. Organic solar cells, therefore, display non-ideal JV-curves. Here, we present a closed-form analytical expression for the JV-curves of organic solar cells, based on the model in reference [1]. The expression is able to reproduce simulated JV-curves for a wide range of mobilities, generation rates and recombination parameters. Most importantly, the model delivers a novel figure of merit α to express the balance between free charge recombination and extraction in low mobility photoactive materials. This figure of merit is shown to determine critical device parameters such as the apparent series resistance and the fill factor. We also find α to be related to the parameter θ as defined in reference [2], showing that the approaches published in [1] and [2] are closely related. With that, we can accurately reproduce the gradual decrease of the fill factor with increasing recombination coefficient, decreasing mobility and increasing thickness.

[1] U. Würfel, D. Neher, A. Spies, S. Albrecht, Nat Commun 2015, 6, 6951 [2] D. Bartesaghi et al., Nat Commun 2015, 6, 7083

CPP 49.3 Thu 10:15 H40

Design Rules for Organic Donor-Acceptor Heterojunctions: Pathway for Charge Splitting and Detrapping — •Carl Poelking and Denis Andrienko — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Organic solar cells rely on the conversion of a Frenkel exciton into free charges via a charge-transfer state formed on a molecular donor-acceptor pair. These charge-transfer states are strongly bound by Coulomb interactions and yet efficiently converted into charge-separated states. A microscopic understanding of this process, though crucial to the functionality of any solar cell, has not yet been achieved. Here we show how long-range molecular order and interfacial mixing generate homogeneous electrostatic forces that can drive charge separation and prevent minority carrier trapping across a donor-acceptor interphase. Comparing a variety of small-molecule donor-fullerene combinations, we illustrate how tuning of molecular orientation and interfacial mixing leads to a trade-off between photovoltaic gap and charge-splitting and detrapping forces, with consequences for the design of efficient photovoltaic devices.

[1] J. Am. Chem. Soc., 2015, **137**, 6320-6326

[2] Nature Materials, 2015, **14**, 434-439

CPP 49.4 Thu 10:30 H40

Investigation of the hybrid charge transfer state at ZnO/organic interfaces — •Fortunato Piersimoni[1], Stefan Zeiske[1], Johannes Benduhn[2], Raphael Schlesinger[3], Norbert Koch[3], Koen Vandewal[2], and Dieter Neher[1] — [1]Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany — [2]Institut für Angewandte Photophysik, Technische Universität Dresden, Dresden, Germany — [3]Institut für Physik & IRIS, Adlershof Humboldt-Universität zu Berlin, Berlin, Germany

This contribution aims to study the Charge Transfer States (CTS) in hybrid systems based upon organic small molecules and ZnO. Those systems were investigated by means of spectrally resolved electroluminescence (EL) and external quantum efficiency (EQE). The presence of Hybrid CTSs is proven by the appearance of a distinct peak in the EL and EQE spectra located below the energy gap of the molecules or ZnO. The energy gap (Egap) between the ZnO conduction band and the donor HOMO was tuned either by varying the ZnO work function through self-assembled monolayers of polar molecules, or by employing organic donors with different HOMO energy. The correspondence between the EL peak position and the Egap attributes this emission to radiative recombination between an electron on the ZnO and a hole on the organic material. Notably all samples displayed a linear relation between the maximum of the EL spectrum and the 2/3 power of the electric field F, in accordance to the confinement of the HCTS in a rectangular electrostatic potential well, implying a certain degree of delocalization perpendicularly to the donor/acceptor interface.

CPP 49.5 Thu 10:45 H40

PBDT[2F]T: Insight into the Secrets of a Wide Band-Gap Polymer with 7% Power Conversion Efficiency — •Julien Gorenflot[1,2], Andreas Paulke[3], Fortunato Piersimoni[3], Federico Cruciani[2], Dieter Neher[3], Pierre M Beaujuge[2], and Frédéric Laquai[2] — [1]Max Planck Institut für Polymerforschung, Mainz, Germany — [2]Universität Potsdam, Potsdam, Germany — [3]King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia

PBDT[2F]BT:fullerene blends exhibit performance up to 75% higher than the reference P3HT:PCBM solar cells [1]. Using femto- to microsecond transient absorption, we investigate the origin of those outstanding properties. We find that geminate recombination losses of photogenerated charge carriers are nearly absent in PBDT[2F]BT:fullerene blends. Field-dependent measurement as well as morphological and energy levels characterization reveal efficient and field-independent charge generation, enabling excellent short-circuit current and fill factor. Strikingly, this outstanding generation is achieved in spite of a rather low offset between the polymer's excitons and the blend's charge transfer state energy levels, which allows for an open circuit voltage as high as 0.9 V. Replacing the fluorine substituents by hydrogen in those polymers results in only moderate performances, thus highlighting the importance of molecular design. This is discussed in terms of energy levels and blends morphology.

[1] J. Wolf et al., Chem. Mater. 27, 2015

15 min. break

CPP 49.6 Thu 11:15 H40

The Meaning of Charge Carrier Density in Charge Extraction Experiments — •Juliane Kniepert, Edgar Nandayapa, and Dieter Neher — University of Potsdam, Potsdam, Germany

Charge extraction experiments are a powerful tool to extract important information on the charge carrier dynamics, such as the effective charge carrier mobility and the order and coefficient of nongeminate recombination, from charge carrier densities under steady state conditions. However, it is often neglected that the extracted carrier density in these experiments is highly sensitive to the actual carrier distribution in the device, which can be very inhomogeneous due to high carrier injection at the contacts, imbalanced mobilities or fast recombination. This is particularly true for organic solar cells, which usually have thin active layers and low intrinsic carrier densities. These conditions may lead to an erroneous interpretation of the results. We show with numerical simulations and experiments how the extracted carrier density is influenced by intrinsic (mobility, recombination coefficient, injection barriers) and extrinsic (layer thickness, illumination, bias) parameters. From these results we deduce experimental conditions for which reliable values for the carrier density, mobility and recombination coefficient can be obtained.

CPP 49.7 Thu 11:30 H40

Rapid non-geminate recombination in organic solar cells — •Jona Kurpiers[1], John Love[1], Christopher Proctor[2], Thuc-Quyen Nguyen[2], and Dieter Neher[1] — [1]Institute of Physics and Astronomy, Soft Matter Physics, University of Potsdam, Germany — [2]Department of Chemistry & Biochemistry, University of California, Santa Barbara, USA

In the last years a dramatic increases in the efficiency of solution processed bulk heterojunction (BHJ) solar cells have been reported. However, the fundamental processes involved in the conversion of absorbed photons to free charges are still not fully understood. In this work, we use time delayed collection field (TDCF) experiments with exceptionally high time resolution to investigate the charge carrier dynamics in polymer-fullerene and small molecule-fullerene systems. TDCF experiments reveal rapid non-geminate recombination on the 20 ns time-scale, even for charge carrier densities comparable to one sun illumination. This loss becomes significantly accelerated at higher pulse fluences for the polymer-fullerene device. To identify the reason for this rapid loss, the recombination dynamics were further investigated on devices with different thicknesses. It is concluded that the primary reason for the nongeminate loss observed at the short time scale in the polymer blend is recombination of charges close to the contacts. In the small-molecule system however, the loss mechanism differs completely. Specifically, we find a rapid filling of traps on short time scales. Our work shows evidence that these rapid loss channels are essential to understand and can dramatically affect device operation.

CPP 49.8 Thu 11:45 H40

Temperature dependent competition between different recombination channels in organic heterojunction solar cells — •Theresa Linderl, Ulrich Hörmann, Sergej Beratz, Mark Gruber, Stefan Grob, Alexander Hofmann, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg

A modification of the Shockley-Queisser theory is presented with a special focus on constellations, where a linear extrapolation of the temperature dependence of the open circuit voltage V_{OC} results in the optical gap of the absorber rather than in the intermolecular charge transfer (CT) gap. Depending on the electronic coupling strength between donor and acceptor molecules, either singlet or CT recombination is dominant in different temperature regimes. These regimes are separated by a transition temperature T_{tr} that is, in the case of small energy level offset and weak electronic coupling, around 300 K or even below. For α-sexithiophene (6T)/diindenoperylene (DIP) solar cells with elevated substrate temperature during 6T deposition the linear extrapolation of the temperature dependent V_{OC} yields a value of 2.07 eV, whereas the extrapolation for the device evaporated at room temperature results in a value of 1.90 eV. Heating the substrate during 6T deposition leads to a molecular configuration at the interface where the coupling between donor and acceptor molecules is strongly reduced compared to the device evaporated at room temperature. This results in a transition temperature well below room temperature which is confirmed by temperature dependent electroluminescence measurements.

CPP 49.9 Thu 12:00 H40

Ambipolar Charge Transfer In Single-Wall Carbon Nanotube Based Bulk-Heterojunctions — •Michael Auth[1], Andreas Sperlich[1], Florian Späth[2], Tobias Hertel[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg — [2]Institute of Physical and Theoretical Chemistry, Julius Maximilian University of Würzburg, — [3]Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg

The exceptional electrical conductivity of Single-Wall Carbon Nanotubes (SWNT) makes them potentially interesting to improve charge transport in organic photovoltaics (OPV). Additionally, their near infrared absorption bands can improve the spectral response of conventional polymer-fullerene bulk-heterojunctions. Until now, only few OPV devices containing purified semiconducting SWNTs were reported regarding the charge transfer properties of solar cell absorbers. For this study we prepared highly purified semiconducting (6,5)-SWNT samples, which we investigated in combination with known OPV donors and acceptors, namely the fullerene acceptor PC$_{60}$BM and the conjugated polymer P3HT. Using Electron Paramagnetic Resonance, we found specific signatures for charge carriers localized on either SWNTs, P3HT or PC$_{60}$BM and revealed the potential ambipolarity of SWNTs, leading to either hole transfer from PC$_{60}$BM or electron transfer from P3HT. Furthermore our measurements confirmed exceptional SWNT purity, with respect to doping, dangling bonds or catalyst residue. In conclusion, we see a high application potential of (6,5)-SWNTs in OPV and, generally, in optoelectronic devices.

CPP 49.10 Thu 12:15 H40

Influence of the Heterojunction's Interface on the Dynamics of Separated Charges Recombination in Organic Photoactive Materials — •Julien Gorenflot[1,2], Niva Alina Ran[3], Mike Heiber[3], Guillermo Bazan[3,4], Thuc-Quyen Nguyen[3,4], and Frédéric Laquai[1,2] — [1]Max Planck Institut für Polymerforschung, Mainz, Germany — [2]King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia — [3]University of California Santa Barbara, Santa Barbara, California, United States — [4]Faculty of Science King Abdulaziz University, Jeddah, Saudi Arabia

A recent study has indicated that the energetic density of shallow trap states, specifically at the interface between the electron donor and the electron acceptor, could be responsible for the apparent high recombination order observed in organic photoactive blends [1]. In order to elucidate this issue, we carried out investigations on a material system that allows for well-controlled donor/acceptor interactions. Films of the small-molecule donor, H1, can be processed such that H1 molecules are either stacking with their pi-face perpendicular or parallel to the substrate. By evaporating a layer of the acceptor molecule C60 on the films, we study the effect of molecular orientation at the donor/acceptor interface on charge recombination using transient absorption spectroscopy. We compare the two bilayer systems to a bulk heterojunction also using H1, which is expected to have a mixture of face-on and edge-on donor/acceptor interactions as well as a much larger interface area. [1] J. Gorenflot et al., J. Appl. Phys.115, 144502 (2014)

CPP 49.11 Thu 12:30 H40

Resonant GISAXS on ternary thin film systems — •Mihael Coric[1], Nitin Saxena[2], Jan Wernecke[3], Stefanie Langner[3], Peter Müller-Buschbaum[2], Michael Krumrey[3], and Eva M. Herzig[1] — [1]Technische Universität München, Munich School of Engineering, 85748 Garching, Germany — [2]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [3]Physikalisch-Technische Bundesanstalt (PTB), Abbestraße 2-12, 10587 Berlin, Germany

Using additives to influence the properties of a material is an extensively used method in material science. It is also an approach to achieve morphological control in binary thin film systems like in organic photovoltaic systems. If the third component is also a polymer the morphological characterization poses a challenge since the sophisticated thin film characterization methods like grazing incidence small angle x-ray scattering (GISAXS) carried out a high x-ray energies can only distinguish between different electron densities. Using x-ray energies near the absorption edges of certain elements contained in the polymers enables a much higher contrast between the different materials, increasing the distinguishability of the different components within the active film of the organic solar cell. However, it is also challenging to interpret the scattering data correctly since some approximations routinely carried out in the theory used for interpretation of hard x-rays are no longer valid. We show our systematic measurements at the sulphur and chlorine edge and explain the advantages we can take out of the measurements to analyze the morphology of this ternary thin film.

CPP 50: Wetting, Nano- and Microfluidics I (joint session CPP/DY, organized by CPP)

Time: Thursday 9:30–12:45 Location: H42

Invited Talk CPP 50.1 Thu 9:30 H42

Provoking liquids to dewet and to slide: About concave drops and hungry droplets — •Karin Jacobs — Experimental Physics, Saarland University, D-66041 Saarbrücken

Usually, liquids exhibit a 'no-slip' boundary condition to a solid substrate, i.e. the atoms or molecules of a liquid that are the closest to the solid substrate are at rest. However, a polystyrene film that moves over hydrophobized (by a self-assembled monolayer of silanes) Si wafers can be provoked to slide, i.e. there is a non-zero interfacial velocity of the fluid in contact with the solid, and friction occurs [1,2]. This implies variations in the energy dissipation mechanisms in these systems and leads to a strikingly different behaviour of fluids in different geometric situations [3-5]: With slip, the dewetting of flat films is faster on solid surfaces (A), Rayleigh-Plateau-type instabilities exhibit an increased dynamics (B) and droplets that were prepared in a non-equilibrium situation can reach equilibrium via a stadium where their topology is concave (C). Yet, why does a liquid slide? Possible explanations including recent findings by scattering methods will be reviewed. Moreover, if more liquids were sliding, would that change things in our everyday life?

[1] O. Bäumchen et al., PRL 113 (2014) 014501; [2] J. D. McGraw et al., Colloid and Interface Science 210 (2014) 13; [3] S. Haefner et al., Nature Comm. 6 (2015) 7409; [4] S. Haefner, O. Bäumchen, K. Jacobs, Soft Matter 11 (2015) 6921; [5] J. McGraw et al., (submitted)

CPP 50.2 Thu 10:00 H42

Soft Levelling: Capillary Relaxation of Thin Liquid Films on Elastic Substrates — •Marco Rivetti[1], Thomas Salez[2], Christine Linne[1], Maxence Arutkin[2], Elie Raphaël[2], and Oliver Bäumchen[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), Göttingen, Germany — [2]UMR Gulliver, CNRS and ESPCI ParisTech, PSL University, Paris, France

A thin liquid film with non-zero curvature at its free surface spontaneously relaxes towards a flat configuration. The flow of this liquid film is driven by Laplace pressure gradients and it is resisted by viscosity. In the last few years the dynamics of this system has been studied experimentally, numerically and analytically. Inspired by recent progresses on the wetting behaviour 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 polystyrene films on polydimethylsiloxane substrates, where the dynamics of the liquid-air interface is monitored using an atomic force microscope. 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 elasto-capillary interaction that is not mediated by the presence of a contact line. We show that the width of the profile scales with the time to the power 1/6, rather than 1/4 which we consistently observed on rigid substrates. A theoretical model that describes the coupled evolution of the elastic-liquid and liquid-air interfaces is also presented.

CPP 50.3 Thu 10:15 H42

Rayleigh-Plateau Instability and Capillary Droplet Propulsion on a Fiber — •Sabrina Haefner[1,2], Michael Benzaquen[3], Oliver Bäumchen[2,4], Thomas Salez[3], Robert Peters[2], Joshua McGraw[1], Elie Raphaël[3], Kari Dalnoki-Veress[2,3], and Karin Jacobs[1] — [1]Saarland University, Dept. of Experimental Physics, D-66041 Saarbrücken, Germany — [2]McMaster University, Dept. of Physics & Astronomy, Hamilton, ON, Canada — [3]PCT Lab, UMR CNRS 7083 Gulliver, ESPCI ParisTech, PSL Research University, Paris, France — [4]Max-Planck Institute for Dynamics & Self-Organization (MPIDS), 37077 Göttingen, Germany

The Rayleigh-Plateau instability (RPI) of a liquid column underlies a variety of hydrodynamic phenomena. Compared to the classical case of a free liquid column, the description of a liquid layer on a fiber requires the consideration of the solid/liquid interface in addition to the free surface. We revisit the RPI of a liquid layer on a solid fiber by varying the hydrodynamic boundary condition at the fiber/liquid interface from no-slip to slip. We find that the growth rate depends on the system geometry and the boundary condition, which is in agreement with theory [1]. In the late stages of liquid column breakup on slip-fibers, a three-phase contact line can be formed on one side of the droplet. The resulting capillary imbalance leads to droplet propulsion, which is studied as a function of temperature and molecular weight [2].

[1] S. Haefner et al., Nat. Commun., 6 (2015), 7409.
[2] S. Haefner et al., Soft Matter, 11, (2015), 6921.

CPP 50.4 Thu 10:30 H42

Rayleigh-Plateau instability of slipping viscous filaments in v-shaped grooves — •Martin Brinkmann[1,3], Tak Shing Chan[1], Ralf Seemann[1], Krishna Khare[2], and Stephan Herminghaus[3] — [1]Experimental Physics, Saarland University, Saarbrücken — [2]Indian Institute of Technology Kanpur — [3]Max Planck Institute for Dynamics and Self-Organisation, Göttingen

Since the seminal works of Rayleigh and Plateau on the break-up of free-standing liquid jets, a large number of studies have addressed the instability of cylindrical interfaces in various experimental settings. The most unstable wavelength λ of a viscous liquid filament wetting the bottom of a v-shaped groove is mainly governed by the slope angle ψ, the contact angle θ of the interface on the solid, and the initial width w of the filament. A linear stability analysis using the method of boundary elements reveals that the characteristic timescale of the decay is affected not only by viscosity, interfacial tension, and geometry. Slip has a substantial effect on the wavelength λ of the fastest growing mode whenever the transverse dimension w of the filaments is comparable or smaller than the Navier slip-length b. In this limit $b/w \to \infty$ we find $\lambda/w \to \infty$ while the timescale τ saturates to a finite lower bound, similar to the case of a free-standing viscous liquid cylinder. In the opposite limit $b/w \to 0$ the corresponding timescale τ of the decay increases only logarithmically with b/w while λ tends to $\sqrt{2}$ times the neutrally stable wavelength λ^*. A linear stability analysis based on long wavelength approximations of the flows agree with the numerical results only for 'flat' filaments $0 < \theta - \psi \ll 1$ with $\lambda^* \gg w$.

CPP 50.5 Thu 10:45 H42

Waves at viscoelastic surfaces — •Julian Kappler and Roland R. Netz — Institut für Theoretische Physik, Freie Universität Berlin, 14195 Berlin, Germany

Waves on water, whose properties depend on gravity and surface tension, are a well-known phenomenon. If there is a surfactant that reacts viscoelastically under compression, like e.g. a biomembrane on water, also another type of surface wave, called longitudinal capillary wave, can exist. On the other hand, on viscoelastic solids there exist Rayleigh waves. These are surface waves which, on a large scale, can be excited by earthquakes, or, on a small scale, can be excited on materials to measure their mechanical properties non-destructively.

We present a unified treatment of all the above waves: We consider a viscoelastic medium covered by a viscoelastic interface and derive a general equation characterizing localized waves at the interface. We show how the aforementioned waves can be derived from this general equation, identify a new surface wave, and discuss how all these waves are interrelated.

Reference: J. Kappler, R. R. Netz. Multiple surface wave solutions on linear viscoelastic media. EPL, 112(1):19002, 2015.

15 min. break

CPP 50.6 Thu 11:15 H42

Non-equilibrium interfacial tension during relaxation — •Markus Bier — Max Planck Institute Int. Sys. and University of Stuttgart, Germany

The concept of a non-equilibrium interfacial tension, defined via the work required to deform the system such that the interfacial area is changed while the volume is conserved, is discussed in the context of the relaxation of an initial perturbation of a colloidal fluid towards the equilibrium state. It is shown that the non-equilibrium interfacial tension is not necessarily positive, that negative non-equilibrium interfacial tensions are consistent with strictly positive equilibrium interfacial tensions and that the sign of the interfacial tension can influence the morphology of density perturbations during relaxation.

References:
[1] M. Bier and D. Arnold, Phys. Rev. E **88**, 062307 (2013).
[2] M. Bier, Phys. Rev. E **92**, 042128 (2015).

CPP 50.7 Thu 11:30 H42

Hydrodynamic cavitation in Stokes flow of anisotropic fluids — •Tillmann Stieger[1], Hakam Agha[2], Martin Schoen[1], Marco G. Mazza[2], and Anupam Sengupta[3] — [1]TU Berlin — [2]MPIDS Göttingen — [3]Massachusetts Institute of Technology

Cavitation is ubiquitous in fluid dynamics, and has significant effects on a wide range of industrial and biomedical applications. Investigations in anisotropic fluids are scarce, and till date, no systematic attempt has been made to study them. Here we report flow-induced cavitation in an anisotropic fluid, studied by combining microfluidic experiments and nonequilibrium molecular dynamics (MD) simulations. Cavitation domains nucleate due to sudden drop in pressure upon flow past a micron-sized obstacle in microchannels, which over time, progressively grows in volume after attaching at the downstream obstacle surface. The inception and growth of cavitation domain ensue in Stokes flow regime. Using MD simulations we study the physical principles governing the cavitation phenomena in nematic liquid crystals (LC), and identify a critical value of Reynolds number Re_{cr} for the cavitation inception that scales inversely with the characteristic order parameter of the LC. Strikingly, the critical Re_{cr} can be as low as $\sim$ 50% of the cavitation threshold in isotropic fluids. Corresponding results for the LC in the isotropic phase and for a Lennard–Jones fluid reveal that the drop in Re_{cr} is a consequence of the long range ordering in anisotropic fluids. The findings suggest that long range ordering, and its tunability, can be potentially applied as a novel control parameter to modulate cavitation inception in anisotropic fluids.

CPP 50.8 Thu 11:45 H42

Sliding Drops - stationary states and large-scale dynamics — •Sebastian Engelnkemper, Markus Wilczek, Svetlana Gurevich, and Uwe Thiele — Institut für Theoretische Physik, Westfälische Wilhelms Universität Münster, Corrensstr. 2, 48149 Münster

The long-wave evolution equation for a liquid film (or Thin-Film-Equation) describes structures including drops and ridges. Including a lateral driving force (e.g., inclined substrate) all structures begin to move and change their shapes. Experiments show this and, in addition, a further instability where large drops emit small satellite drops [1]. Implementing the Thin-Film-Equation in the continuation-toolbox PDE2PATH [2], we analyze the primary bifurcations from a flat film in the case without driving using the mean film height as bifurcation parameter. Then, with lateral driving forces we track sliding drops in dependence of either drop volume or substrate inclination. We analyze the shape changes and compare them to previous 1d results [3]. Finally, we focus on the bifurcation that is responsible for the satellite drops and relate the results of continuation to direct numerical simulations for single drops and ensembles of many drops. [1] T. Podgorski, J.-M. Flesselles, L. Limat, Phys. Rev. Lett. 87, 036102 (2001); [2] H. Uecker, D. Wetzel, J.D.M. Rademacher, arXiv:1208.3112v2 (2012); [3] U. Thiele et al., Phys. Rev. E, 64, 061601 (2001).

CPP 50.9 Thu 12:00 H42

Autophobing drops, fuelled by oil/water interfacial chemistry — Bijoyendra Bera, •Michael Duits, Dirk van den Ende, Martien Cohen Stuart, and Frieder Mugele — University of Twente, Enschede, The Netherlands

We report a hitherto not observed wetting phenomenon, namely the retraction of a drop after deposition on a solid substrate, caused by an interfacial reaction between cations in the aqueous drop and fatty acids in the ambient oil. We investigate how this process depends on the concentrations of the reactants, the chain lengths of fatty acid and alkane solvent, and the solid substrate material. We demonstrate with contact angle and AFM measurements that deposition of amphiphilic molecules on the solid takes place only after assembly at the oil-water interface. Deposition of material by the moving contact line leads to an increasingly hydrophobic local substrate and a concomitant increase in contact angle, which we call autophobing. This phenomenon is observed both on mica and on silica substrates, for several fatty acids and alkane solvents. The time-dependent contact angle can be described with a theoretical model in which the adsorption reaction at the oil-water interface is rate-limiting, and transfer to the solid is determined by a mass flux balance (similar to a Langmuir Blodgett transfer). The ensuing time-dependent oil-water and solid-oil interfacial tensions then produce the evolution of the contact angle.

CPP 50.10 Thu 12:15 H42

Compact nanosensors probe microdroplets — •Julian Schütt[1], Felix Zörgiebel[1,2], Bergoi Ibarlucea[1,2], Sebastian Pregl[1,2], Daijiro Nozaki[1], Walter Weber[2,3], Thomas Mikolajick[2,3,4], Larysa Baraban[1,2], and Gianaurelio Cuniberti[1,2] — [1]Max Bergmann Center of Biomaterials and Institute for Materials Science, Dresden University of Technology, Budapesterstrasse 27, 01069 Dresden, Germany — [2]Center for Advancing Electronics Dresden, 01062 Dresden, Germany — [3]Namlab GmbH, Nöthnitzerstraße 64, 01187 Dresden, Germany — [4]Institute for Semiconductors and Microsystems, TU Dresden, 01062 Dresden

Smart combination of nanosensors and droplets based reactors represents a powerful tool for monitoring and high throughput analysis of the kinetics of biological and chemical reactions, staying miniaturized, highly sensitive and optically label-free. Here we present a first demonstration of droplets microfluidics with the compact silicon nanowire field effect transistor (SiNW FET) on a single chip for in flow electrical detection of aqueous reactor-drops. Apart from detection events, we chemically probe the content of numerous droplets in a row as independent events (up to ten thousands), and resolve the pH values and ionic strength of the solution, resulted in a change of a source-drain current through the nanowires. Optic-less and noninvasive measurements of these parameters in aqueous droplets have a great impact on the area of biodetection and bioanalytics as a high throughput screening tool for pathogens, drug assays, and evaluation of the enzymatic activities.

CPP 50.11 Thu 12:30 H42

Stability of emulsions against coalescence and transport: Influence of surfactants — •Birte Riechers[1,2], Philipp Gruner[2], Florine Maes[1,2], and Jean-Christophe Baret[1,2] — [1]CNRS, Univ. Bordeaux, CRPP, UPR 8641, Pessac, France — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Monodisperse aqueous droplets within emulsions become evermore attractive for use as separate microreactors in pharmaceutical and biotechnological applications [Theberge *et al.*, Angewandte 2010]. These applications need constant experimental conditions inside the droplets. To date stabilization against coalescence is mainly obtained using surfactants. Surfactants also affect the solubility of solutes inside the continuous oil phase, thereby restricting their use [Gruner *et al.*, Curr. Opin. Colloid Interface Sci. 2015]. Microfluidic tools provide insight into the mechanisms of interfacial stabilization:
Here we perform a complete analysis of the adsorption kinetics of a surfactant typically used in droplet-based microfluidic applications. We combine pH measurements at the micronscale and coalescence experiments in droplet-based microfluidics with bulk measurements to show that the kinetics of the transport of molecules across interfaces directly relates to those of interfacial stabilisation. Combining all information, we derive a simple model of adsorption in the kinetic-limited regime and show that two interfaces are only stabilized against coalescence for surfactant concentrations which are close to or above the critical micellar concentration.

CPP 51: Glasses (joint session CPP/DY, organized by DY)

Time: Thursday 9:30–13:00 Location: H48

Invited Talk CPP 51.1 Thu 9:30 H48

A new look at atomic tunneling systems in glasses containing isotopes with nuclear quadrupol moments — •Andreas Reiser — Kirchhoff Institut für Physik, Universität Heidelberg, INF 227, 69120 Heidelberg, Germany

The physical properties of disordered materials at low temperatures are governed by atomic or molecular tunneling systems. The standard tunneling model explains many properties such as thermal conductivity and heat capacity well. In dynamic experiments for example dielectric susceptibility measurements or polarization echo experiments clear deviations from the standard tunneling model are observed. In particular, the strong influence of nuclear moments inherent in tunneling atoms was proven experimentally recently. We will discuss the mechanism that leads to the interplay of nuclear moments and atomic tunneling systems and will show that at ultra low temperatures a new type of relaxation process enabled by nuclear moments is present. Contrary to previous assumptions this process governs the energy relaxation of the tunneling systems in the limit of lowest temperatures rather than the one phonon process.

CPP 51.2 Thu 10:00 H48

Theoretical investigation of mechanism and statistical properties of a model two-dimension silica glass. — •Projesh Kumar Roy[1] and Andreas Heuer[2] — [1]Graduate school of chemistry, Institute of physical chemistry , Correnstrasse 28/30, D-48149, Muenster — [2]Institute of physical chemistry , Correnstrasse 28/30, D-48149, Muenster

The discovery of 2D silica glass [1] [2] has offered a realistic description of random network theory of silica glass structure; debated for over 80 years[3]. This extremely thin material consists of two layers of silica and exhibits 2D properties in all phases. In the glass phase, the silica network shows a log-normal ring distribution with a typical microstructure or triplet distribution. For simulations two different models based on a Soft - core Yukawa potential[4] and a Stillinger Weber type multi-body potential, have been employed with a binary mixture of silicon and oxygen type particles. After energy minimization, the defect free structures were identified and their ring statistics were compared with the experiment. Going beyond the experiment, the observations can be related to the underlying local energies. Furthermore, two major mechanisms turn out to be responsible for creating various random networks. On this basis a new Monte-Carlo algorithm is proposed for generating random networks of defect free 2D silica.

[1] Heyde M., Shaikhutdinov S., Freund H.-J., Chem. Phys. Lett. 550, 1 (2012). [2] Huang P. Y. et al, Nano Lett. 12, 1081 (2012). [3] Zachariasen W.H., J. Am. Chem. Soc. 54, 3841 (1932). [4] Mendez-Maldonado G.A., et al., J. Chem. Phys. 137, 054711 (2012).

CPP 51.3 Thu 10:15 H48

Relevance of Nuclear Quadrupoles to the Low Temperature Dielectric Properties of Glasses — •Annina Luck, Benedikt Frey, Wiebke Scholz, Guido Homann, Anne Zeissner, Nils Hauff, Philipp Wesp, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, 69120 Heidelberg

The standard tunneling model based on two level systems describes many properties of solids at low temperatures. Over the years the measurements of dielectric and acoustic properties have, however, shown significant deviations from predictions made by this model. Despite enormous efforts these deviations are yet unexplained.
One aspect which is missing in the prediction of low frequency dielectric properties by the tunneling model is the relevance of nuclear spins, which has been proven to be important in dielectric polarization echo experiments at 1 GHz. Despite of this, modelling the consequences of this effect on the low frequency dielectric and acoustic susceptibility has proven difficult.
In order to experimentally investigate the role of nuclear quadrupoles in the dielectric susceptibility we have investigated multiple glass samples containing elements with different quadrupole moments in a wide frequency range spanning from Hz to GHz.
We have found clear indications for a novel nuclear spin driven two level system relaxation process at very low temperatures.

CPP 51.4 Thu 10:30 H48

Glass transition and stable glass formation of carbon tetrachloride — •Yeong Zen Chua[1], Michael Tylinski[2], Mark D. Ediger[2], and Christoph Schick[1] — [1]Institute of Physics, University of Rostock, Rostock 18051 Germany — [2]Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53706 USA

There have been attempts to find correlations between the ability to form stable glasses and general characteristic of the materials. It was argued that asymmetric molecules, which allow anisotropic packing on the surface during deposition, are a prerequisite for stable glass formation. This leads to the question whether symmetric molecules can form stable glasses. Carbon tetrachloride (CCl_4) is an ideal molecule to verify this hypothesis, since the molecule is pseudo spherical with no orientation. On the other side, the formation of stable glasses is thought to be mediated by a highly mobile surface layer. So it might be expected that CCl_4, as a small and simple organic molecule, has enhanced mobile surface layer and thus increases its ability to form stable glasses. These conflicting factors lead to our investigation of CCl_4 glasses produced by physical vapor deposition with *insitu* AC chip nanocalorimetry. Kinetically stable glasses have been observed to form at substrate temperature around 0.8 T_g, consistent with previous work on stable glass formers. The isothermal transformation of the as-deposited glasses into supercooled liquid state gave further evidence to support the stable glass formation, thus disproving molecular asymmetry as a prerequisite. The glass transition temperature is determined as $T_g = (78\pm2)$ K, which is different from previously reported values.

CPP 51.5 Thu 10:45 H48

Influence of MCM-41 on the dynamical and phase behaviors of aqueous mixtures — •Matthias Sattig and Michael Vogel — Institut für Festkörperphysik, TU Darmstadt, Hochschulstraße 6, 64289 Darmstadt, Germany

The dynamics of aqueous mixtures in bulk and confinement is a topic of great interest. Two model systems, which exhibit rather different behavior upon varring water concentration are propylene glycol- and propylene glycol monomethyl ether-mixtures. This was attributed to the different ability of both alcohols to form hydrogen bonds in neat systems and in aqueous mixtures. The formation of H-bond networks can be altered by geometrical confinement, whose surface interacts with the guest molecules and provides spatially restriction. Here we provide temperature dependent deuteron-NMR data of heavy water in mixture with PG, PGME or di-PGME confined in mesoporous MCM-41 in a broad dynamic range. We examin the rotational autocorrelation using stimulated echo experiments and spin-lattice-relaxation. The latter exhibits a typical minimum in its relaxation time T_1, below which several relaxation processes could be identified in the different mixtures, supporting the idea of a phase separation in confinement, that was proposed in QENS [1] and dielectric [2] investigations. We compare our results with the dynamics of water [3] and glycerol confined in the same material to discuss similarities and differences relating to the influence of confinement on the dynamics of neat and mixed systems. [1] Swenson et al., JCP, 141, 214501, 2014 [2] Elamin et al., PCCP, 17, 12978, 2015 [3] Sattig et al., JCPL, 5, 174 - 178 , 2014

CPP 51.6 Thu 11:00 H48

Spatio-temporal Correlations of Glass-forming Systems in Terms of Coupled Energy Landscapes — •Carsten Schroer[1,2] and Andreas Heuer[1,2] — [1]Westfälische Wilhelms-Universität Münster, Institut für physikalische Chemie, Corrensstraße 28/30, 48149 Münster, Germany — [2]NRW Graduate School of Chemistry, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany

The concept of the potential energy landscape is an effective tool for the physical description of supercooled liquids in the vicinity of the glass-transition. In this framework, typically small elementary systems are studied for which a strong correlation between its thermodynamic state and its dynamics can be found[1]. The transfer of these insights to macroscopic systems can be achieved by regarding the larger system as a superposition of elementary systems. The observed finite-size effects of the structural relaxation time contain important information about the coupling between these subsystems[2].

In this talk we discuss the impact of this coupling mechanism on the occurrence of spatio-temporal correlations, measured by four-point correlation functions. The results obtained by our model are compared with numerical data obtained by molecular dynamics simulations. We demonstrate that this model, based on the energy landscape of the small system plus the coupling, is sufficient to describe complex behavior of glass-formers.

[1] A. Heuer, *J. Phys.: Condens. Matter* **20**, 37 (2008).

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

CPP 51.7 Thu 11:15 H48

Colloidal monodisperse hard ellipsoids — •Patrick Pfleiderer[1], Stefan Schütter[2], Nicolai Sänger[2], Matthias Klein[2], and Andreas Zumbusch[2] — [1]Department of Physics, University of Konstanz, 78457 Konstanz, Germany — [2]Department of Chemistry, University of Konstanz, 78457 Konstanz, Germany

The hard sphere system has been generating hundreds of publications per year for the past decades. The focus of attention has recently been shifted towards anisotropic particles, as rotational degrees of freedom have been identified as key for progress in statistical mechanics models and engineering alike. One prominent puzzle is the violation of Stokes-Einstein(-Debye) relations near the glass transition.

The next obvious simple system besides spheres is the hard ellipsoid system. It lends itself to theoretical descriptions and simulations. While an experimental technique to prepare colloidal poly(methyl methacrylate) (PMMA) ellipsoids exists since the 1990s, little progress has been made towards an establishment anywhere near the 'fruit fly' hard spheres. This is due to the difficulties in endowing several desired properties simultaneously to the system: mass-density and refractive-index matching, hard-core interactions, long-term stability etc. We present the first 3D hard ellipsoid system which meets all these goals, fluorescently labeled with a unique core-shell structure [1], polydispersity as low as 3%, and study the interplay of rotational and translational degrees of freedom approaching the colloidal glass transition.

[1] M.K. Klein, N. Saenger, S. Schuetter, P. Pfleiderer, and A. Zumbusch, Langmuir 30, 12457 (2014).

15 min. break

CPP 51.8 Thu 11:45 H48

Electron bombardment induced cation transport in an ion conducting glass — •Anneli Hein, Jan Wiemer, and Karl-Michael Weitzel — Fachbereich Chemie, Philipps-Universität Marburg

The bombardment induced ion transport (BIIT) technique has been developed for measuring ionic conductivities and activation energies for ion hopping. The original version is based on attaching a cation beam to the sample (cation-BIIT) inducing the transport of such cations towards a grounded backside electrode. In the current work the BIIT technique is extended to electron bombardment (e- - BIIT). Here a low energy electron beam has been attached to a mixed sodium and potassium conducting borosilicate glass mounted on a single grounded backside electrode. Attachment of the electrons to the surface induces cation transport towards this surface. In the first part of the experiment current-voltage curves have been measured. The specific conductivities as well as the activation energy for ion hopping derived agree with cation-BIIT data. In the second part of the experiment we have performed a long term electron bombardment of the glass sample at -25 eV. Ex situ - after the bombardment - the sample has been analyzed by time-of-flight secondary ion mass spectrometry (ToF-SIMS). The depth profiles obtained from the ToF-SIMS analysis clearly demonstrate that sodium has been neutralized at the front side of the glass sample due to the recombination of electrons with sodium ions. Reduction of the less noble potassium ions appears to be suppressed. The electrochemical implications of this observation will be discussed.

CPP 51.9 Thu 12:00 H48

Residual stresses in glass forming systems — •Gaurav Prakash Shrivastav[1], Pinaki Chaudhuri[2], and Jürgen Horbach[1] — [1]Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany — [2]The institute of Mathematical Sciences, Chennai, India

When a sheared glass is allowed to relax, stress does not decay to zero but tends towards a finite value. How the resulting residual stress is spatially distributed in the system is only poorly understood, especially in the case of a sheared system with shear bands. Also, the effect of different shear rates, with which the initial glass is deformed, and the effect of the amount of strain present in the initial deformed glass on the residual stress distribution are open issues.

In the present work, we study, using molecular dynamics simulations, relaxation of stresses in a sheared model glass former. We first deform a binary glass forming Lennard-Jones mixture by shearing it with a constant strain rate. Then, we switch of the shear in different regimes of the stress-strain curve and allow the system to relax. We find that the amount of residual stress in the system depends on the initial strain before the shear cessation. By looking at the spatially resolved mean square displacement of particles, we find that the residual stress remains localized in regions where the shear band has been present before. We also find that the deformed glass has higher Poisson's ratio than the undeformed glass, consistent with previous observations.

References

[1] I Binkowski, G. P. Shrivastav, J. Horbach, S. V. Divinski, G. Wilde arXiv:1506.03031 (2015).

CPP 51.10 Thu 12:15 H48

Nonlinear Microrheology of Supercooled Liquids in Terms of an Effective Temperature — •Carsten Schroer[1,2] and Andreas Heuer[1,2] — [1]Westfälische Wilhelms-Universität Münster, Institut für physikalische Chemie, Corrensstraße 28/30, 48149 Münster, Germany — [2]NRW Graduate School of Chemistry, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany

We perform computer simulations of a fragile model glass-former in which a single particle is driven by an external force through the liquid. Thereby, we track the path the system takes through its underlying Potential Energy Landscape (PEL) and aim for understanding how this is altered by the external field[1,2] and how the altering is related to the nonlinear responses of dynamic quantities. In this talk, we show that, for strong forces, the thermodynamic state and the local kinetics of the system is altered by the external force in a similar way as an increase of the (bath) temperatures. This behavior gives rise to the definition of an *effective temperature* that turns out to be characterized by a single force and temperature-independent parameter only, even for bath temperature below the computer glass transition. Combining these observations enables us to derive scaling relations for the nonlinear mobility and the diffusive properties of the tracer particle that are tested with our numerical data [3].

[1] C. F. E. Schroer, A. Heuer, *J. Chem. Phys.* **138**, 12A518 (2013).
[2] C. F. E. Schroer, A. Heuer, *Phys. Rev. Lett.* **110**, 067801 (2013).
[3] C. F. E. Schroer, A. Heuer, *J. Chem. Phys.* (accepted) (2015).

CPP 51.11 Thu 12:30 H48

Nonlinear Microrheology of Supercooled Liquids in Terms of an Effective Temperature — •Carsten Schroer[1,2] and Andreas Heuer[1,2] — [1]Westfälische Wilhelms-Universität Münster, Institut für physikalische Chemie, Corrensstraße 28/30, 48149 Münster, Germany — [2]NRW Graduate School of Chemistry, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany

We perform computer simulations of a fragile model glass-former in which a single particle is driven by an external force through the liquid. Thereby, we track the path the system takes through its underlying Potential Energy Landscape (PEL) and aim for understanding how this is altered by the external field[1,2] and how the altering is related to the nonlinear responses of dynamic quantities.

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[1] C. F. E. Schroer, A. Heuer, *J. Chem. Phys.* **138**, 12A518 (2013).
[2] C. F. E. Schroer, A. Heuer, *Phys. Rev. Lett.* **110**, 067801 (2013).
[3] C. F. E. Schroer, A. Heuer, *J. Chem. Phys.* (accepted) (2015).

CPP 51.12 Thu 12:45 H48

Potential energy landscape analysis of sheared glass-forming systems — •Markus Blank-Burian and Andreas Heuer — Institut für Physikalische Chemie, WWU Münster, Deutschland

We performed molecular dynamics simulations of small binary Lennard-Jones mixtures ($65 \leq N \leq 1040$) under constant shear rates and at very low temperature ($T = 0.01$) as well as above T_g. We also performed shear reversal simulations.

In previous work on unsheared systems it was shown, that most of the physical properties of macroscopic systems are already encoded in small systems. We can show that finite size effects have only limited influence on major observables of the sheared system at $N = 130$.

For the analysis of the sheared system, we perform energy minimization using the strain as an additional variable. We then use this information to identify inherent structures (IS) and metabasins (MB) from the trajectories. The IS have zero strain and are therefore comparable to the unsheared system.

From the resulting statistical data we gain a microscopic understanding of macrorheological phenomena like the initial stress overshoot as well as shear thinning in the plastic flow regime from a potential energy landscape perspective.

CPP 52: Focus: Two Dimensional Functional Materials I

Organizers: Armin Goelzhaeuser (Universität Bielefeld), Holger Frauenrath (EPFL Lausanne)

Two-Dimensional Functional Materials are characterized by having one dimension in the molecular or atomic length scale, whereas the other two dimensions are extended. This 2D geometry allows a use as functional components or hybrids in electronics, fluidics, sensing or filtration. The Focus Session will cover a variety of materials, their fabrication processes, properties and applications. A particular emphasis is laid on 2D materials whose fabrication includes molecular assembly: 2D polymers, bio membranes, covalent organic frameworks (COFs), functionalized graphene, Carbon Nanomembranes (CNMs) and others.

Time: Thursday 9:30–12:30 Location: H51

Invited Talk CPP 52.1 Thu 9:30 H51

Synthesis of 2D polymers — •Dieter A. Schlüter — ETH Zurich, Department of Materials, Zurich, Switzerland

Two-dimensional materials (2DM) are sheet-like entities and of great interest for their manifold properties. Famous representatives are graphene, boronitride or molybdenum disulfide. 2DMs are often provided by nature or are obtained under harsh conditions. Such conditions exclude the synthetic arsenal of organic chemistry to be used for rational sheet creation, sheet structure variation and sheet engineering on a molecular level. Recently it was shown that covalent monolayer sheets can be easily accessed at room temperature by genuine two-dimensional polymerizations of organic monomers applying simple protocols. They include spreading of monomers at an air/water interface or crystallizing them into layered single crystals followed by metal complexation or light-induced growth reactions. These growth reactions result in macroscopic sheets of considerable mechanical strength. Some of them are composed of planar repeat units over their entire expanse and were introduced as synthetic two-dimensional polymers (2DP). Particularly in view of the ease of synthesis and the high level of structure control during polymerization we consider this the onset of a major research activity with serious applications at the horizon. Synthetic sheets and 2DPs will increasingly complement graphene and other known sheets. The contribution addresses strategic, synthetic and analytical issues and provides a view into future.

Invited Talk CPP 52.2 Thu 10:00 H51

Carbon nanomembranes as a platform for engineering of functional 2D materials — •Andrey Turchanin — Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — Jena Center for Soft Matter (JCSM)

Carbon nanomembranes (CNMs) are ultrathin molecular sheets (~1 nm) which can be generated via electron, ion or photon induced crosslinking of aromatic self-assembled monolayers. Similar to graphene or other atomically thin 2D materials (hBN, MoS2, etc.) they possess mechanical integrity and therefore can be transferred from their original substrates onto new substrates, fabricated as suspended sheets or stacked into van der Waals heterostructures with a precise control over their thickness. Their physical and chemical properties can be tuned via an appropriate choice of molecular precursors or their post modification, providing a flexible platform for engineering of functional 2D materials. In this talk, some examples of these materials and their applications in devices will be presented. These examples include: (i) biofunctional and photoactive CNMs; (ii) gratings for matter-wave interferometry; (iii) growth of graphene with adjusted electronic and structural properties; (iv) chemical functionalization of graphene and MoS2 field-effect devices; (v) novel hybrid 0D/2D layered materials.

CPP 52.3 Thu 10:30 H51

Functional Carbon Nanosheets From Amphiphilic Hexayne Precursors At Interfaces — •Bjoern Schulte, Stephen Schrettl, and Holger Frauenrath — École Polytechnique Fédérale de Lausanne, Institute of Materials, Laboratory of Macromolecular and Organic Materials, Station 12, 1015 Lausanne, Switzerland

The access to functional two-dimensional carbon nanomaterials remains challenging despite intensive research. Established synthetic routes follow either top-down or bottom-up strategies. Top-down approaches yield materials with a high degree of structural perfection but are mostly limited to small-scale production. Bottom-up approaches promise to be better scalable, but often preclude chemical functionalization of carbon nanomaterials due to the high temperatures required for the carbonization of the precursors. Recently, our group reported on a new approach to obtain two-dimensional carbon nanomaterials from hexayne amphiphiles as molecular precursors. The amphiphilic precursors contain a segment of sp-hybridized carbons that is highly reactive and undergoes carbonization upon irradiation with UV light at room temperature. These mild conditions allow to transfer the chemical functionality of the precursor to the carbon nanomaterial. Based upon the formation of a dense self-assembled monolayer of hexayne precursors at the air-water-interface amphiphilic carbon nanosheets with a thickness of less than 2 nm and lateral dimensions of square centimeters are obtained. Further extending our work, we will provide a more detailed study of the properties of hexayne amphiphiles at interfaces.

CPP 52.4 Thu 10:45 H51

Touchless finger motion tracking with humidity sensitive 1D Photonic Crystals — •Katalin Szendrei — Max Planck Institute for Solid State Research, Stuttgart, Germany — Ludwig Maximilians Universität, München, Germany

1D Photonic Crystals (1D PCs) are periodic multilayered nanostructures exhibiting a photonic band gap - a forbidden spectral range for photons propagating through the nanostructure. These structures are promising candidates for smart optical detectors as the structural color can be dynamically changed by external chemical, physical or biological stimuli. Herein we present 1D PCs fabricated by bottom up assembly from colloidal metal oxide nanoparticles and colloidally stable suspensions of antimony phosphate 2D nanosheets, which show an ultrasensitive response to local humidity changes caused by the moisture induced swelling of the nanosheets. Integrated into a PC, a resulting full spectrum color change is indicative of ultrahigh sensitivity towards water vapor. The combination of a high selectivity, high reproducibility and response time in the subsecond time scale allowed us to detect minute humidity changes. As the human finger is surrounded by a humid atmosphere, finger positions and motions can be tracked and indicated by color changes of the BS in realtime under touchless conditions. These experiments suggest a new device architecture as alternative to the common touchscreen technology. With the touchless technology, the disadvantages of hygienic aspects, mechanical vastage could be avoided, while at the same time the user receives a direct feedback of the finger motion through the optical answer of the display.

15 min. break

CPP 52.5 Thu 11:15 H51

Making atomically thin perforated nanomembranes — •Andreas Winter[1], Yasin Ekinci[2], Armin Gölzhäuser[3], and Andrey Turchanin[1,4] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena — [2]Laboratory for Micro- and Nanotechnology, Paul Scherrer Institute, 5232 Villigen, Switzerland — [3]Faculty of Physics, Bielefeld University, 33615 Bielefeld — [4]Jena Center for Soft Matter, 07743 Jena

Two-dimensional (2D) materials like graphene, hexagonal boron nitride or carbon nanomembranes (CNMs) have recently attracted enormous interest due to their potential use in electronics, chemical and biological sensors, nanofilters, and hybrid materials. Lithographic patterning of 2D materials allows to form nanostructures required e.g. in filter or nanosensoric applications. In this respect, extreme UV interference lithography (EUV-IL) provides possibilities for large-scale and high resolution patterning with an ultimate size limit in the 10 nm-range. Here we present the preparation of atomically thin perforated nanomembranes and their characterization with a helium ion microscope (HIM), which is especially suitable to image topographic features of freely suspended membranes. Examples for the area-selective crosslinking of self-assembled monolayers and resist-based lithography as well as the use of perforated membranes for interferometry of massive molecules will be given.

CPP 52.6 Thu 11:30 H51

Transfer of covalently modified large area graphene — •Felix Rösicke[1,2], Marc A. Gluba[1], Guoguang Sun[3], Karsten Hinrichs[3], Jörg Rappich[1], and Norbert Nickel[1] — [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 by p-aminophenyl residues from the respective diazonium salt (p-aminobenzenediazonium tetrafluoroborate). Subsequently, these amino functional groups were modified by activated p-nitrobenzoic acid via an amidation reaction. All processes were performed before and after the transfer of graphene onto SiO2 coated silicon wafers. After the electrochemical grafting the samples were characterized using Raman backscattering and infrared spectroscopic ellipsometry measurements. The data show that similar results were obtained for grafting of graphene on Cu foil and SiO2 coated silicon. Moreover, electrochemically functionalized graphene on Cu was successfully transferred to other substrates without damaging the functional groups. Considering the variety of possible diazonium cations, this opens the possibility to the use of modified graphene as tailored modular building block for specific surface functionalization.

CPP 52.7 Thu 11:45 H51

Gas permeation through carbon nanomembranes — •Vahe Chinaryan[1], Sergey Shishatskiy[2], Jan Wind[2], Xianghui Zhang[1], Henning Vieker[3], Polina Angelova[3], Volker Abetz Abetz[2], André Beyer[1], and Armin Gölzhäuser[1] — [1]Physics of Supramolecular Systems, University of Bielefeld, 33615 Bielefeld, Germany — [2]Institute of Polymer Research, Helmholtz-Zentrum Geesthacht, 21502 Geesthacht, Germany — [3]CNM Technologies GmbH, 33609 Bielefeld, Germany

The gas permeation characteristics of carbon nanomembranes (CNMs) from self-assembled monolayers are reported. CNMs are 1 nm thick sheets, made by the cross-linking of molecular monolayers. CNMs were placed onto polydimethylsiloxane (PDMS) membranes to determine the gas permeation characteristics for single- and multi-layers of CNMs. CNMs made from different molecules having thicknesses from 0.6 nm up to 1.2 nm were investigated with regard to the permeation of different gases (He, H2, CO2, O2, N2,...). The CNM-PDMS composites were also characterized by X-ray photoelectron spectroscopy and helium-ion microscopy. The permeation characteristic of CNMs indicates a molecular-sieve-like transport mechanism which can be attributed to molecular-sized channels in CNMs. Additionally, the permeance of CNMs is adjustable by varying the length of the precursor molecules, i.e. the thickness of single-layer CNMs. Multilayers of CNMs show a permeation that differs significantly from single-layer CNMs, possibly due to the diffusion of the permeating molecules in between the CNM layers.

CPP 52.8 Thu 12:00 H51

Covalent functionalisation of pristine and vacancy defective single-walled carbon nanotubes with diisocyanates — •Mariana Kozlowska — University of Bialystok, Ciolkowskiego Str. 1K, 15-245 Bialystok, Poland

Mechanical properties and thermal stability of polyurethanes can be improved with the addition of small amounts (0.1 wt%) of carbon nanotubes (CNTs). The formation of such hybrid systems may be proceeded via covalent grafting of polyurethanes to reactive isocyanate groups located onto the sidewalls and at the ends of CNTs. The isocyanate groups can be attached to the CNT surface during the reaction between the aromatic diisocyanates with the carboxyl or hydroxyl groups on its surface.

The present work focuses on the structural properties of aromatic diisocyanates (4,4-methylene diphenyl diisocyanate, toluene-2,4-diisocyanate) covalently attached to the pristine and defective (single vacancy and 5-8-5 divacancy) SWCNT(10,0). The detailed analysis of the results obtained using static DFT calculations in combination with Car-Parrinello molecular dynamics simulations at 300 K will be shown.

The authors gratefully acknowledge the financial support of the University of Bialystok within the Grant for Research of Young Scientists, grant number BMN 175.

CPP 52.9 Thu 12:15 H51

Quantitative SFM-Imaging of Graphene Functionalization: Toward Well-Defined Wrappings for Multivalent Virus Interactions — •Mohammad Fardin Gholami[1], Daniel Lauster[2], Kai Ludwig[3], Julian Storm[2], Benjamin Ziem[3], Nikolai Severin[1], Christoph Böttcher[3], Jürgen P. Rabe[1], Andreas Herrmann[2], Rainer Haag[3], and Mohsen Adeli[3] — [1]Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin — [2]Institut für Biologie, Humboldt-Universität zu Berlin — [3]Institut für Chemie und Biochemie, Freie Universität Berlin

Multivalency is widely used by nature to control biological interactions. Therefore, we also considered it for the design of a new generation of anti-viral drugs. Two-dimensional materials are promising carriers for multivalency. Graphene, in particular, is very robust yet chemically rather inert and therefore it is difficult to control the density distribution of its functionalization. We employed Scanning Force Microscopy (SFM) in quantitative imaging mode to investigate the functionalization of thermally reduced graphene oxide sheets and further used the sheets for the inhibition of the vesicular stomatitis virus (VSV) as a model virus. The functionalization of the sheets was carried out using a [2+1] nitrene cycloaddition reaction at ambient conditions. SFM imaging reveals a high density and homogenous distribution of the functionalization, depending on reaction conditions. Moreover, it allows to gain insight into the interaction of the multivalently functionalized sheets with VSV depending on the type and density of the functionalization.

CPP 53: Biomaterials and Biopolymers II (joint session BP/CPP/MM, organized by MM)

Time: Thursday 11:45–13:00 Location: H52

CPP 53.1 Thu 11:45 H52

Stimuli responsiveness of electron irradiated gelatin — •Stefanie Riedel[1,2], Emilia I. Wisotzki[1,2], Katharina Apel[1], Wolfgang Knolle[1], and Stefan G. Mayr[1,2] — [1]Leibniz-Institut für Oberflächenmodifizierung, Leipzig — [2]Fakultät für Physik und Geowissenschaften, Universität Leipzig

Stimuli responsive materials have attracted considerable interest during the past years due to their potential use in sensor and actuator applications. They are designed to transform small external stimuli e.g. temperature and humidity changes into a significant response.

While a large number of alloys or synthetic polymers are well-established at this point, we explore the potential of the biomaterial gelatin to respond to humidity changes. We demonstrate how irradiation with high-energetic electrons allows fine-tuning of the response. In addition, this treatment enhances thermal stability providing high attractiveness for biomedical applications.

CPP 53.2 Thu 12:00 H52

Langzeitverhalten von Seide und "Selbstheilung" — •Jan Rosigkeit[1], Igor Krasnov[1] und Martin Müller[1,2] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität Kiel — [2]Institut für Werkstoffforschung, Helmholtz-Zentrum Geesthacht

Durch Streckexperimente haben wir mechanische Eigenschaften des biologischen Nanokomposits Seide unter Verwendung eines Modells aus der linearen viskoelastischen Theorie [1] über lange Zeiten bestimmt. Wir stellen fest, dass sich die mechanischen Eigenschaften der Seide auf langen Zeiten "fraktional" viskoelastisch ("Memory"-Effekt) beschreiben lassen.

Seidenfasern können sich in zwei Zuständen befinden. Einer dieser Zustände ist ein stabiler Zustand der nicht vorgestreckten Faser. Der andere Zustand wird durch äußere Krafteinwirkung hervorgerufen, wodurch eine vorgestreckte Faser entsteht. Wir haben experimentell gezeigt, dass der Übergang vom vorgestreckten zum Anfangszustand in einer nassen Umgebung innerhalb von 24 Stunden stattfindet. Der vorgestreckte Zustand ist daher ein metastabiler Zustand. [2]

[1] W. Glöckle und T. Nonnenmacher, Macromol., **24:**6426-6434 (1991).

[2] J. Rosigkeit, Bachelorarbeit, Christian-Albrechts-Universität Kiel (2014).

CPP 53.3 Thu 12:15 H52

Fractional dynamics in silk — •Igor Krasnov[1], Tilo Seydel[3], and Martin Müller[2] — [1]IEAP, Universität Kiel, Germany — [2]Institute of Materials Research, HZG, Germany — [3]ILL, Grenoble, France

Structural relaxations in humid silk fibers exposed to tensile stress have been observed to take place on a very wide range of time scales from a few milliseconds to several hours. The time-dependence of the measured tensile force following a quasi-instantaneously applied external strain on the fibers can be understood in terms of a fractional viscoelastic relaxation function introducing memory effects by which the mechanical state of a fiber depends on its tensile history. [1] An analog fractional relaxation also gives rise to the subdiffusion observed on picosecond time scales, which governs the mobility of the amorphous polymer chains and adsorbed water on the molecular level. The reduction of the subdiffusive memory effect in stretched fibers compared to native fibers is consistent with the higher order of the polymers in the stretched state.

[1] I. Krasnov, T. Seydel, and M. Müller, Phys. Rev. E 91, 042716 (2015)

CPP 53.4 Thu 12:30 H52

Mechanical properties of branched actin filaments — •Mohammadhosein Razbin[1], Martin Falcke[3,4], Panayotis Benetatos[5], and Annette Zippelius[1,2] — [1]Georg August University — [2]Max Planck Institute for Dynamics and Selforganization — [3]Humboldt University — [4]Max Delbrueck Center for Molecular Medicine — [5]Kyungpook National University

Motile cells on a 2dimensional substrate generate motion by flat membrane protrusion called lamellipodia. Within lamellipodia, actin filaments are generated by branching off existing ones, giving rise to branched network structures. We investigate the force-extension relation of branched actin filaments, grafted on an elastic substrate at one end and pushing with the free ends against a flat and stiff wall. We compute the thermal fluctuation of the endpoints and the resulting entropic forces on a membrane, restricting the fluctuations of the endpoints. The entropic forces are shown to depend sensitively not only on the persistence length but also on the geometry of the structure. It depends on branch point position and filament orientation, being most pronounced for intermediate tilt angles and intermediate branch point positions. We describe filament networks without crosslinkers to focus on the effect of branching. We compare properties of branched and unbranched networks. The ratio of the network average of the force per branched filament to the average force per unbranched filament exhibits compression dependence and may go up to about 4.5 in networks with a narrow orientation distribution. With orientation distributions measured in lamellipodia, it is about 2.

CPP 53.5 Thu 12:45 H52

Tension, Balance and Flex: Auxetic periodic tensegrities — •Myfanwy Evans — TU Berlin, Berlin, Germany

We present here a class of triply-periodic tensegrity structures that have a negative Poisson's ratio: they are auxetic. These theoretical materials are derived from periodic rod packings or more general periodic filament packings with a dilatant property. We show that these chiral tensegrity structures are periodically rigid but affinely flexible. The affine flex leads to isotropic expansion or contraction. A parallel can be drawn between these tensegrity structures and woven materials with elastic filaments, which also display an auxetic behaviour. Such materials are an exciting target for functional materials and biomaterials, from metal-organic frameworks to woven polymeric or filamentous structures.

CPP 54: Hybrid and Perovskite Photovoltaics IV (joint session CPP/DF/DS/HL, organized by HL)

Time: Thursday 14:45–18:30 Location: H2

CPP 54.1 Thu 14:45 H2

Synthesis of perfectly oriented and micrometer-sized MAPbBr3 perovskite crystals for thin film photovoltaic applications — •Nadja Giesbrecht[1], Johannes Schlipf[2], Andreas Binek[1], and Pablo Docampo[1] — [1]Department of Chemistry and Center for NanoScience (CeNS), University of Munich (LMU), Butenandtstr. 5-13, 81377 Muenchen,Germany — [2]Lehrstuhl fuer Funktionelle Materialien, Physik-Department, Technische Universitaet Muenchen, James-Franck-Str. 1, 85748 Garching, Germany

Wide band-gap perovskites such as methylammonium lead bromide (MAPbBr3) are interesting materials for photovoltaic applications due to their potentially high open-circuit voltage. However, the fabrication of high quality planar films has not been investigated in detail for this material. We report a new synthesis approach for the fabrication of bromide based perovskite planar films based on the control of the deposition environment. The correlation of photocurrent and perovskite crystal properties in photovoltaic devices is studied. We achieve dense layers with large and perfectly oriented crystallites, as confirmed with grazing incidence wide angle X-ray scattering (GIWAXS). This represents the first solution-processed MAPbBr3 perovskite film with such a high degree of order. The current output was found to depend on crystal order in the perovskite film with internal quantum efficiencies approaching unity. Hence, our work not only gives a new pathway to tune morphology and crystal orientation, but demonstrates its importance for planar perovskite solar cells.

CPP 54.2 Thu 15:00 H2

Structural properties of hybrid perovskites from first principles — •Jingrui Li[1], Jari Järvi[1,2], Hugo Levard[1], and Patrick Rinke[1] — [1]Aalto University, Helsinki, Finland — [2]University of Helsinki, Finland

Hybrid perovskites have received rapidly growing interest in recent years as promising photoactive materials in emergent photovoltaic technologies. We present a first-principles analysis of the atomistic structure of the methylammonium lead triiodide ($\mathrm{CH_3NH_3PbI_3}$) perovskite in this work, with a particular focus on the orientation of $\mathrm{CH_3NH_3^+}$ cations and its interplay with the inorganic matrix. Relativistic density functional theory calculations were performed using the all-electron local-atomic-orbital code `FHI-aims`. Our results indicate that (i) the lattice constants obtained by incorporating the long-range van der Waals interactions (using the Tkatchenko-Scheffler method) in the PBE exchange-correlation functional agree well with experiments; (ii) hydrogen bonding between the ammonium group and the $\mathrm{I^-}$ anions plays the decisive role in the position of the $\mathrm{CH_3NH_3^+}$ cation and the shape of the $\mathrm{PbI_3^{2-}}$ framework; (iii) the reorientation of $\mathrm{CH_3NH_3^+}$ is limited due to the high barriers (~ 80 meV). Based on these findings we establish a self-consistent multiscale model, in which the energetically favorable alignment of $\mathrm{CH_3NH_3^+}$ dipoles in the material is determined by combining classical electrostatics and statistics with structure relaxation in DFT. Our procedure produces representative “pseudo random” methylammonium lead triiodide supercells that will form the basis of further first-principles work.

CPP 54.3 Thu 15:15 H2

Micrometer size grains of hybrid perovskite through rapid melting procedure — •Oleksandra Shargaieva, Felix Lang, Jörg Rappich, Carola Klimm, Manuela Klaus, Bernd Rech, and Norbert Nickel — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Kekuléstr. 5, 12489 Berlin (Germany)

Interest in hybrid perovskites as an absorber has flared since the first successful attempts in dye solar cells (DSCs) and continues to grow as a promising material for solar cells application. The usage of such compounds is often associated with the opportunity to substitute existing materials due to the remarkable simplicity of the production process and its low costs. On the other hand, solution based processing of solid perovskite layers often includes difficulties with crystallization, which could result in the formation of grain boundaries. This type of crystalline defect has a strong impact on the performance of devices and tends to lower the power conversion efficiency.

In our work, we propose a new solvent-free approach to produce perovskite type compounds based on its melting process. This simple technic allows to obtain bulk material with grain sizes of several micrometers. Melting process enables the control of the crystallization of hybrid perovskite and by that suppresses grain boundaries formation. Furthermore, the procedure was optimized and successfully introduced into thin-film fabrication. Consequently, melting of perovskites gives a possibility to decrease non-radiative recombination and therefore, can improve the performance of the device.

CPP 54.4 Thu 15:30 H2

J-V Hysteresis Observed in Methylammonium Lead Halide Perovskite Films at Different Voltage Scales — •Martina Stumpp, Raffael Ruess, Jonas Horn, Jan Tinz, Christoph Richter, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen, GERMANY

Hysteresis in the current-voltage curves of methylammonium lead halide films deserves detailed investigation because it can affect their applicability in perovskite solar cells. In the current study, J-V hysteresis of $CH_3NH_3PbI_3$ and $CH_3NH_3Pb(I_{0.95}Br_{0.05})_3$ prepared via different established deposition techniques was studied in a symmetric contact geometry of microstructured gold electrode arrays on SiO_2/Si wafers. The measured J-V characteristics showed a different behavior of hysteresis depending on the applied voltage range. Residual currents at zero applied bias were observed following positive or negative poling showing persistent polarization of the perovskite films. At higher bias voltages, additional inverted hysteresis loops were measured pointing at a decrease in barrier height and width at blocking perovskite/metal contacts, presumably caused by migrating iodide ions. The net J-V characteristics in this voltage range can be simulated by two diodes operated back-to-back. Time-dependent studies were performed to analyze the decay of the different observed polarization phenomena in the films during either short-circuit or continuous sweeping of the bias.

CPP 54.5 Thu 15:45 H2

Water infiltration in methylammonium lead iodide: fast and inconspicuous — •Christian Mueller[1,2,3], Bernd Epding[2,3], Tim Helder[2,3], Michael Sendner[2,3], Annemarie Pucci[2,3], Wolfgang Kowalsky[1,2,3], and Robert Lovrincic[1,3] — [1]IHF, TU Braunschweig, Germany — [2]KIP, Universität Heidelberg, Germany — [3]InnovationLab, Heidelberg, Germany

Extensive research efforts over the last few years led to a significant increase in power conversion efficiency of organometal-halide perovskite (such as $\mathrm{CH_3NH_3PbI_3}$) solar cells up to over 20%. However, our understanding of physical/chemical processes in the material lags behind device progress. For instance, the impact of water on $\mathrm{CH_3NH_3PbI_3}$-based devices, despite being well documented, is still not well understood and as such remains controversial.

Herein we use IR spectroscopy in controlled atmosphere to demonstrate that water infiltration into $\mathrm{CH_3NH_3PbI_3}$ occurs much faster and at much lower humidity than previously thought. We show that the exposure of $\mathrm{CH_3NH_3PbI_3}$ to ambient environment leads to an increase of the photocurrent by more than one order of magnitude in lateral devices. Based on transient photocurrent measurements we speculate that the effect is associated with enhanced proton conduction when light is combined with water and oxygen exposure. Our results suggest that water infiltration plays an important role in the optoelectronic properties of $\mathrm{CH_3NH_3PbI_3}$ based devices, well beyond the known water triggered degradation processes[1].

[1] C. Mueller et al., Chem. Mater., 27 (22), p. 7835-7841, 2015

CPP 54.6 Thu 16:00 H2

Graphene on Hybrid Solar Cells: from Silicon and Perovskite towards Tandem Solar Cells — •Felix Lang, Matthias Zellmeier, Marc A. Gluba, Steve Albrecht, Jörg Rappich, Lars Korte, Bernd Rech, and Norbert H. Nickel — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium Photovoltaik, Kekuléstr. 5, 12489 Berlin, Germany

A variety of hybrid solar-cell architectures require the deposition of a highly transparent and conductive contact. However, deposition techniques for conventional transparent conductive oxides typically degrade the topmost organic layers. A non-destructive wet transfer process of large area graphene from the growth substrate onto the desired sample is the clear choice to tackle this challenging problem.

Here, we present for the first time the implementation of graphene on hybrid crystalline silicon/P3HT solar cells. Despite identical V_{OC} and superior external quantum efficiency, device performance is limited by graphene sheet resistance. To overcome this limitation we combined in-situ graphene doping with an absorber with a higher band gap. Both measures reduce the impact on the device performance.

Implementation of graphene on the perovskite $CH_3NH_3PbI_3$ therefore enabled a semi-transparent device concept showing superior internal quantum efficiency compared to conventional Au-contacted solar cells. The graphene contact enabled an optical sub-band gap transmission of around 60 % for the complete device. This paved the way for the development of a four terminal crystalline silicon/perovskite tandem solar cell with a power conversion efficiency of 13.2 %.

CPP 54.7 Thu 16:15 H2

GW for transition metal perovskites — •Zeynep Ergonenc, Bongjae Kim, Peitao Liu, Georg Kresse, and Cesare Franchini — University of Vienna, Faculty of Physics and Center for Computational Materials Science

The ab initio calculation of quasiparticle (QP) energies beyond density functional theory is a technically and computationally challenging problem. In condensed matter physics the most widely used approach to determine QP energies is the GW approximation. The GW method has been widely applied to many elemental and binary semiconductors, but its application to more complex compound such as perovskites is less abundant. In this work we apply the GW technique to transition metal perovskites with different occupancies of d orbitals. We show that much care must be taken to obtain converge QP band structure in terms of number of unoccupied orbitals and k-points sampling. Accurate extrapolation procedures to the infinite-basis-set limit and infinite-k-point limit are necessary.

30 min. Coffee Break

CPP 54.8 Thu 17:00 H2

Controlling the optical properties of organic/inorganic halide perovskites by means of size and composition — •Verena A. Hintermayr, Lakshminarayana Polavarapu, Alexander S. Urban, and Jochen Feldmann — Chair for Photonics and Optoelectronics, Department of Physics, Ludwig-Maximilians-Universität (LMU), Amalienstaße 54, 80799 Munich, Germany

Organic/Inorganic halide perovskites display a huge potential for not only photovoltaic, but also light emitting applications. In order to improve the efficiency and functionality of applications based on this material a better control of their optical properties is desirable. Here, we present a general colloidal synthesis method for the preparation of hybrid organic/inorganic halide perovskite nanocrystals (NCs) with different size and composition. We have prepared highly stable perovskite NCs that show strong quantum confinement and NCs that exhibit bulk like optical properties. We additionally investigate the tunability of the optical properties of the NCs by systematically modifying their halide content (I, Br and Cl). This work opens up a simple synthetic route for the preparation of perovskite NCs with controllable dimensionality and composition.

CPP 54.9 Thu 17:15 H2

Dynamics and nature of photo-excited carriers in $(CH_3NH_3)PbI_3$ organic-inorganic perovskite — •Daniel Niesner[1,2], Haiming Zhu[1], Tyler J. S. Evans[1], Bryan J. Kudisch[1], Prakriti P. Joshi[1], Kiyoshi Miyata[1], M. Tuan Trinh[1], Manuel Marks[1], and X.-Y. Zhu[1] — [1]Department of Chemistry, Columbia University, New York, NY 10027, USA — [2]Festkörperphysik, FAU Erlangen-Nürnberg, D-91058 Erlangen, Germany

Thin film solar cells based on organic-inorganic perovskites are the rising star in photovoltaics. The photophysics and transport mechanism behind the outstanding device performance remain a matter of debate. I will present the results of a study on carrier dynamics in vapor-deposited thin films of $(CH_3NH_3)PbI_3$, combining time-resolved two-photon photoemission, transient absorption, and photoluminescence.

After optical excitation with sufficient photon energy ($\geq$ 2.15 eV), highly excited electrons relax quickly ($\leq$ 0.3 ps) to a region of the conduction band with a low density of states, located 0.3 eV above the band minimum. In parallel, polaron formation takes place on a time scale of 0.28 ± 0.04 ps, matching the time scale of cation motion. Polaronic screening suppresses further energy relaxation and thermalization. The polaron maintains a significant excess energy for more than 60 ps.

The excess energy can be utilized to overcome energy barriers at grain boundaries and contacts. Harvesting it directly would result in a solar cell with an efficiency exceeding the Shockley-Queisser limit.

CPP 54.10 Thu 17:30 H2

Infrared spectroscopic study of vibrational modes and water infiltration in methylammonium lead halide perovskites — •Michael Sendner[1,2], Christian Mueller[1,2,3], Tobias Glaser[1,2], Annemarie Pucci[1,2], Wolfgang Kowalsky[1,2,3], and Robert Lovrincic[2,3] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg — [2]InnovationLab GmbH, Heidelberg — [3]Institut für Hochfrequenztechnik, TU Braunschweig

The interactions of the organic cation with the inorganic lattice in organo-metallic halide perovskites influence the vibrational properties of the cation which can be measured in the mid infrared (IR) spectral region. We determined the infrared optical properties of different methylammonium lead halide perovskite films ($CH_3NH_3Pb(I/Br/Cl)_3$) and derived the full dielectric function [1]. The peaks of the vibrational modes are assigned by means of the comparison with MP2 calculated modes of the free methylammonium cation. The influence of the inorganic cage and the processing is discussed. Furthermore, we utilize IR spectroscopy to investigate the influence of water onto perovskite thin films. We show that the infiltration of water into $CH_3NH_3PbI_3$ appears much faster and at much lower humidity than previously known [2]. We suggest a molecular picture of this infiltration where water molecules have a strong impact on the hydrogen bonding between the methylammonium cations and the surrounding Pb-I cage. [1] T. Glaser et al. J. Phys. Chem. Lett. 2015, 6 (15), 2913-2918 [2] C. Müller et al. Chem. Mater., 2015, 27 (22), 7835-7841

CPP 54.11 Thu 17:45 H2

Temperature and excitation density dependence of two-photon photoluminescence of perovskite CH3NH3PbBr3 — •Heiko Linnenbank[1], Michael Saliba[2], Lili Gui[1], Bernd Metzger[1], Giuseppe Nasti[2], Jeanette Kadro[2], Anders Hagfeldt[2], Michael Graetzel[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Laboratory of Photonics and Interfaces, École polytechnique fédérale de Lausanne, Station 6, 1015 Lausanne, Switzerland

Recently solution processed organometallic halide perovskites have attracted much attention due to their simple processability, strong light absorption and favorable emission properties, which promises the realization of efficient on chip lasers. While several studies have been focused on one-photon excited luminescence processes like amplified spontaneous emission or lasing, only less attention has been paid to two-photon excited processes. In contrast to the usually expected quadratic dependence upon the excitation density in the case of two-photon photoluminescence, we rather measure a 4th power dependence at room temperature in the case of CH3NH3PbBr3. Such an excitation density dependence is a strong hint for a biexcitonic or exciton collision processes, which are rather unlikely at room temperature. To clarify the origin of the 4th power dependence, we investigate the form as well as the excitation density dependence of the photoluminescence spectra with respect to the sample temperature, revealing a suppression of the 4th power dependence with decreasing temperature.

CPP 54.12 Thu 18:00 H2

Dark field photoluminescence and scanning electron beam measurements on single organic/inorganic halide perovskites of varying geometry and composition — •Alexander Richter, Verena Hintermayr, Lakshminarayana Polavarapu, Alexander Urban, and Jochen Feldmann — Chair for Photonics and Optoelectronics, Department of Physics, Ludwig-Maximilians-Universität (LMU), Amalienstaße 54, 80799 Munich, Germany

During recent years organic/inorganic halide perovskites have become a promising candidate for photovoltaic applications and also show a huge potential for light emitting applications. In case of two dimensional crystals quantum confinement affects the optical properties. Here, we present results on individual nanocrystals. Perovskites fabricated with varying halide content and geometry are embedded in a polymer matrix film to prevent degradation. Dark field photoluminescence and scanning electron beam measurements on individual spots of the sample are carried out. This yields a direct link between shape, halide composition and photoluminescence of these particles.

CPP 54.13 Thu 18:15 H2

Luminescence blue-shift with decreasing size of perovskite needles. — •Amala Elizabeth and Katrin F.Domke — Molecular Spectroscopy Department,Max Planck Institute for Polymer Research, Mainz, 55128, Germany

Despite revolutionizing the photovoltaic industry by helping create highly efficient thin film solar cells, many intrinsic properties of organometallic halide perovskites still remain unknown. A complete understanding of the interplay of size, structure and electronic nature in determining the optical properties of thin film perovskites is crucial to fully exploit them for solar cell applications.

We studied methylammonium lead iodide perovskite thin films of ordered needles of varying submicron size. Energy-dispersive X-ray and IR spectroscopies reveal that the needles are chemically identical. While crystallinity is preserved in all samples, XRD and Raman spectra show a relative increase in the crystalline lead iodide content with decreasing needle size. Interestingly, we observe a blue-shift of 40 meV in both luminescence peak position and UV-vis absorption onset with decreasing needle size. Here, we discuss possible origins of the unexpected band gap increase with decreasing perovskite needle size, such as methyl ammonium cation orientational ordering [1] and lead iodide content [2].

References:

1. C. Quarti et al., J.Phys.Chem Lett. 5 (2014), 279-284.
2. Q.Shen et al., Nano Lett. 14 (2014), 4158-4163.

CPP 55: Symposium SYAD: Anomalous Diffusion in Complex Environments (BP/CPP/DY, organized by BP)

Time: Thursday 15:00–17:45 Location: H15

Invited Talk CPP 55.1 Thu 15:00 H15

Phenomenology of Collective Chemotaxis in Artificial and Living Active Matter — •Ramin Golestanian — University of Oxford

The non-equilibrium dynamics of active particles that send and receive chemical signals could lead to enhanced and/or anomalous diffusion, as well as spontaneous formation of interesting structures and patterns due to the long-range nature of the interactions. We examine theoretically the consequences of this interaction, and present some results that exemplify the type of emergent properties that could result from them, including: spontaneous formation of small stable clusters or “molecules” that can exhibit functionality that depends on geometry, collective chemotaxis in a solution of catalytically active colloids that could lead to cluster formation, aster condensation, and spontaneous oscillations, swarming - in the form of a comet - of light-induced thermally active colloids with negative Soret coefficient due to a shadowing interaction, and collective behaviour of a colony of cells that divide and interact chemotactically.

Invited Talk CPP 55.2 Thu 15:30 H15

First-passage times of Markovian and non Markovian random walks in confinement — •raphael Voituriez — CNRS/ Université Pierre et Marie Curie, Paris, France

The first-passage time is a key quantity for evaluating the kinetics of various processes, and in particular chemical reactions involving ”small” numbers of particles. A striking example is given by gene transcription, where specific proteins search for target sequences on DNA. I will present asymptotic results which enable the evaluation of the distribution of the first-passage time to a target site for a wide range of random processes in confined domains, and show how these results can be extended to non Markovian processes.

Invited Talk CPP 55.3 Thu 16:00 H15

Cytoskeleton organization as an optimized, spatially inhomogeneous intermittent search strategy — •Heiko Rieger, Yannick Schröder, and Karsten Schwarz — Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany

The efficiency of intracellular transport of cargo from specific source to target locations is strongly dependent upon molecular motor assisted motion along cytoskeleton filaments, microtubules and actin. Radial transport along microtubules and lateral transport along the filaments of the actin cortex underneath the cell membrane are characteristic for cells with a centrosome. Here we show that this specific filament organization for ballistic transport in conjunction with intermittent diffusion realizes a spatially inhomogeneous intermittent search strategy that is in general optimal for small thicknesses oft he actin cortex. We prove optimality in terms of mean first passage times for three different, frequently encountered intracellular transport tasks: 1) the narrow escape problem (e.g. transport of cargo to a synapse or other specific region of the cell membrane), 2) reaction kinetics enhancement (e.g. binding of two mobile reaction partners within the cell), 3) the reaction-escape problem (e.g. release of cargo at a synapse after intracellular vesicle pairing). Since homogeneous search strategies could only be realized by completely filling the search volume with randomly oriented cytoskeleton filaments, our results indicate that living cells realize optimal search strategies for various intracellular transport problems *economically* through a spatial cytoskeleton organization that involves only small amounts of randomly oriented actin filaments.

15 min break

Invited Talk CPP 55.4 Thu 16:45 H15

Ergodicity violation and ageing in living biological cells — •Ralf Metzler — Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany

In 1905 Einstein formulated the laws of diffusion, and in 1908 Perrin published his Nobel-prize winning studies determining Avogadro’s number from diffusion measurements. With similar, more refined techniques the diffusion behaviour in complex systems such as the motion of tracer particles in living biological cells is nowadays measured with high precision. Often the diffusion turns out to deviate from Einstein’s laws.

This talk will discuss the basic mechanisms leading to anomalous diffusion as well as point out the physical and biological consequences, for instance, in gene regulation or cargo transport in cells. In particular the unconventional behaviour of non-ergodic, ageing systems will be discussed. Concrete examples include the motion of submicron and nanoprobes in biological cells, uncrowded and crowded lipid membranes, as well as interacting many particle systems.

Invited Talk CPP 55.5 Thu 17:15 H15

Anomalous diffusion within cells — Sarah Klein[1,2], •Cecile Appert-Rolland[1], and Ludger Santen[2] — [1]Laboratory of Theoretical Physics, CNRS, Univ. Paris-Sud, Bat 210, 91405 Orsay, France — [2]Fachrichtung Theoretische Physik, Univ. des Saarlandes D-66123 Saarbrücken, Germany

Within cells, various objects (vesicles, organelles,...) need to be transported. Some processive molecular motors get attached to these objects (or cargos) to form a complex that will have a stochastic motion along a network of microtubules. Intriguingly, there is some evidence that this motion results from a tug-of-war between teams of motors that pull in opposite directions.

A stochastic model for cargo-motors complex allows us to study the properties of the resulting motion along a single microtubule. We find some anomalous diffusion, both subdiffusive or superdiffusive depending on the timescale. Interestingly, such anomalous diffusion has indeed been observed experimentally. I will discuss the importance of fluctuations in the dynamics, and present some hypotheses why nature chose such a transport process to carry cargos through the crowded interior of cells.

[Klein, Appert-Rolland, Santen, EPL 107 (2014) 18004,
Eur. Phys. J. Special Topics 223 (2014) 3215,
EPL 111 (2015) 68005]

CPP 56: Organic-Inorganic Systems III: Electronic Structure (organized by O)

Time: Thursday 15:00–18:00 Location: S051

Invited Talk CPP 56.1 Thu 15:00 S051

Electrostatic Design of Organic Materials and Hybrid Interfaces — •Egbert Zojer — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010-Graz, Austria

In hybrid organic/inorganic interfaces collective electrostatic effects often determine electronic properties like the relative alignment of electronic states, adsorption-induced changes in the work-function, XPS shifts and ballistic transport properties. Here, we suggest ways of intentionally employing these effects for realizing new types of electrostatically designed nanoscopic materials. This includes the development of a modular and versatile toolbox for realizing complex interfacial structures like monolayer quantum-cascades or quantum-well structures. It also comprises the use of polar adsorbates on layered van-der Waals bonded materials like graphene or layered semiconductor structures with the aim of locally concentrating charge carriers for an adsorbate-driven patterning of conductive channels. Finally, I will address possibilities for electrostatically designing the energy landscape of self-assembled three-dimensional organic networks with possible applications in charge carrier separation or carrier injection.

CPP 56.2 Thu 15:30 S051

Electronic structure of charge transfer salts: application of self-interaction corrected density functional theory — •Torsten Hahn[1], Torsten Hahn[2], and Torsten Hahn[2] — [1]Institute for Theoretical Physics, TU Freiberg, 09599 Freiberg, Germany — [2]IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

We present our experimental and theoretical results on novel Picene/F4TCNQ and Manganese-Phthalocyanine/F4TCNQ donor / acceptor systems. We apply the recently developed Fermi-orbital based approach for self-interaction corrected density functional theory (FO-SIC DFT) to these materials and compare the results to standard DFT calculations [1,2,3]. Further we compare the theoretical results with experimental data obtained by photoemission spectroscopy. We focus our analysis on the comparison of orbital eigenvalues, ionization potentials and the magnitude of the ground state charge transfer. We show that for weakly bound donor / acceptor systems the FO-SIC approach delivers results closer to experiment compared to standard DFT calculations.

[1] T. Hahn et al., J. Chem. Phys. (accepted: AIPID 029546JCP).
[2] M. R. Pederson, A. Ruzsinszky, and J. P. Perdew, J. Chem. Phys. 140, 121103 (2014).
[3] M. R. Pederson, J. Chem. Phys. 142, 064112 (2015).

CPP 56.3 Thu 15:45 S051

Structural and electronic properties of organic charge-transfer complexes on Ag(111) — •Kathrin Müller[1,2], Nico Schmidt[1], Michael Grunst[3], Rene Riedel[3], Milan Kivala[3], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, Netherlands — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]Department of Chemistry and Pharmacy, University Erlangen-Nürnberg, Germany

The use of organic molecules in electronic devices is gaining increasing interest due to their low cost, flexibility and easy processability. However, organic molecules often show weak intermolecular interactions limiting the electron mobility of organic films. One way to overcome these problems is the use of complementary molecules, which exhibit a strong intermolecular interaction. We employ molecules with complementary functional groups as well as complementary building blocks, e.g. by using electron rich and electron poor building blocks. In this work, we studied the self-assembly and the electronic properties of two molecules containing cyano- and methoxy-groups, respectively, on a Ag(111) surface. The cyano-functionalized molecule exhibits a high electron affinity, while the other one shows a low ionization potential. The investigations of the structural and electronic properties of the individual species as well as the mixed layer were carried out by scanning tunneling microscopy and spectroscopy, X-ray and ultraviolet photoelectron spectroscopy and low-energy electron diffraction. We found that the electronic properties of the mixed layer are changed with respect to the assemblies containing one molecular species.

CPP 56.4 Thu 16:00 S051

Electronic Structure of TIPS-Pentacene on Au(111) — •Arnulf Stein and Petra Tegeder — Physikalisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg, Germany

Functionalized Oligoacenes have moved into the field of view for applications in organic electronic devices during the last years. One representative of this group of organic semiconductors is the triisopropylsilylethynyl-pentacene (TIPS-Pc) which stands out because it combines solubility, self-assembly into π-stacked arrays to enhance intermolecular orbital overlap [1] and vacuum processability [2]. Furthermore it can undergo a singlet fission process [3], which is one possibility to overcome the theoretical Shockley Queisser - Limit. We investigated the TIPS-Pc/Au(111) interface by means of two-photon-photoemission (2PPE) which is one of the most powerful tools to elucidate electronic structures and dynamics of optically excited states at interfaces and within thin films.

[1] J.E. Anthony *et al.*, JACS, 123, 9482 (2001).
[2] A. Gnoli *et al.* J. Phys. Chem. C, 118, 22522 (2014).
[3] A. J. Musser *et al.* Nat. Phys. 11, 352 (2015).

CPP 56.5 Thu 16:15 S051

Charge transport across interfaces between metals and disordered-semiconductors — Philipp Breitegger[1], Markus Krammer[1], Chris Groves[2], and •Karin Zojer[1] — [1]Institute of Solid State Physics and NAWI Graz, Graz University of Technology, Graz, Austria — [2]School of Engineering and Computing Sciences, Durham University, United Kingdom

Injection of charges from the metal contacts into organic semiconductors, i.e., de facto insulators, is crucially determining the performance of organic devices. Reaching an in-depth understanding of fundamental processes occurring when a steady-state electric current passes the interface, is an indispensable step towards truly active control of charge transport, e.g., by manipulating both interface and semiconductor via intentional doping. To conceive a model being strictly based on the injection barrier, the shape of the density of states, and the external bias, we utilize Kinetic Monte Carlo simulations to identify conditions leading to ohmic or space charge limited currents, i.e., currents being exclusively determined by the semiconductor. A fraction of charges entering the semiconductor is immobilized at the interface such that the Fermi level becomes aligned with the semiconductors transport energy at the interface. Owing to this alignment, further carriers are injected resonantly and contribute to the current. On the basis of these findings, we formulate a necessary condition to obtain bulk-limited current irrespective of the injection barrier.

CPP 56.6 Thu 16:30 S051

Characterizing Charge-Transfer Effects at Metal/Organic Interfaces by means of Two-Photon Photoemission — •David Gerbert and Petra Tegeder — Physikalisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg, Deutschland,

Further progress in the field of organic electronic devices requires a fundamental understanding of metal/molecule interactions at the interface between organic semiconducting materials and metal electrodes. These metal/molecule interactions lead to an energetic realignment, including the formation of new states and even bands, which may act as a basis for a improved device performance [1].Two-photon photoemission (2PPE) is a powerful tool which enables the observation of occupied and unoccupied electronic states directly at the interface. Additionally 2PPE experiments can be performed in a time-resolved or angle-resolved manner to gain insights into dynamics of optically excited electronic states and possible delocalized charge-carriers.

In this talk I will show recent results of different adsorbate/metal interfaces indicating adsorption-induced energetic realignment and band formation.

[1] M. Wießner et al., Nat- Commun. 2013, 4, 1514.

CPP 56.7 Thu 16:45 S051

Excitation dynamics at the PTCDA/TiOPc heterointerface on Ag(111) — •Alexander Lerch[1], Frederik Schiller[1,2], and Ulrich Höfer[1] — [1]Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg — [2]Centro de Física de Materiales, San Sebastian, Spain

The charge carrier transport across metal/organic and organic heterointerfaces was investigated by means of time-resolved two-photon photoemission (2PPE). We deposited well defined layers of perylene-3,4,9,10-tetracarboxylic dianhydride (PTCDA) on top of titanylphthalocyanine (TiOPc) on an Ag(111) substrate as model system. An optical parametric oscillator (OPO) provided tuneable pump pulses with photon energies ranging from 1.6 to 2.5 eV. Excitons in PTCDA and TiOPc were excited selectively and the subsequent charge transfer to the metal was monitored by photoemission with 4.3 eV probe pulses. An unoccupied interface state lying 0.3 eV above the Fermi energy arises at the TiOPc/Ag(111) interface. Although a second TiOPc layer is used to form the organic heterostructure and separate the PTCDA from the silver, we observe a resonant enhancement of the interface state for 2.3 eV pump photons, which corresponds to the excitonic HOMO-LUMO transition in PTCDA. We find a time delayed transfer of electrons from PTCDA across the TiOPc layers into the interface state on the time scale of approximately 200 fs. Our results indicate the importance of the interface state for charge carrier dynamics at heterostructures close to the Ag(111) surface.

CPP 56.8 Thu 17:00 S051

Nanoscale Imaging of Charge Carrier and Exciton Trapping at Structural Defects in C_{60} Films — •Christoph Grosse[1], Olle Gunnarsson[1], Pablo Merino[1], Klaus Kuhnke[1], and Klaus Kern[1,2] — [1]Max-Planck-Institut fürr Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]École Polytechnique Fèdérale de Lausanne, 1015 Lausanne, Switzerland

Charge carrier and exciton trapping in organic semiconductors crucially determine the performance of organic (opto-) electronic devices, such as organic field-effect transistors, light-emitting diodes, or solar cells. However, the microscopic origin of the relevant traps generally remains unclear, as most spectroscopic techniques are unable to probe the electronic structure of individual traps and the morphological structure causing them. Here, we employ low-temperature scanning tunneling microscopy (STM) and tunneling spectroscopy as well as tight-binding calculations derived from ab initio calculations to image the localized electronic states arising at structural defects in thin C_{60} films (<10 ML). The spatially and spectrally resolved STM-induced luminescence at these states reveals an enhanced radiative decay of excitons, which is interpreted in terms of the local symmetry lowering and the trapping of excitons by an X-traps. The combined mapping of the STM-induced luminescence, electronic structure, and morphology thus provides new insights into the origin and characteristics of individual exciton traps in organic semiconductors and opens new avenues to study charge carrier and exciton dynamics at molecular scales.

CPP 56.9 Thu 17:15 S051

Theory of excitation transfer in hybrid inorganic/organic systems: Coulomb transfer between semiconductor and molecular layers — •Judith Specht[1], Eike Verdenhalven[1], Sverre Theuerholz[1], Andreas Knorr[1], Marten Richter[1], Bjoern Bieniek[2], and Patrick Rinke[2,3] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Berlin, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [3]Aalto University, Aalto, Finland

Hybrid inorganic/organic systems form a novel class of composite materials with interesting optoelectronic properties. Due to the Coulomb interaction, Wannier-exciton like states in an inorganic semiconductor nanostructure are coupled to Frenkel excitons occurring in organic materials. The considered structure consists of a thin, highly ordered molecular film adsorbed on a semiconductor quantum well. Based on a density matrix theory, we study the Förster-type non-radiative excitation transfer across the hybrid interface. The microscopic input parameters are taken from ab initio caculations for ladder-type quarterphenyl (L4P) molecules on the ZnO($10\bar{1}0$) surface [1]. As a consequence of microscopic momentum selection rules, the coupling strength between the two constituents varies for different coverage densities of the semiconductor surface with molecules.Our findings can be used for optimizing the energy transfer efficiency by modifying the geometry of the hybrid structure.

[1] Verdenhalven et al., Phys. Rev. B **89**, 235314 (2014).

CPP 56.10 Thu 17:30 S051

Photo Switching the Optical Nonlinear Response of a Fulgimide Functionalized Silicon Surface — •Marc Hänsel[1], Christoph Barta[2], Karola Rück-Braun[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg, Germany — [2]Institut für Chemie, Technische Universität Berlin, Germany

Fulgimides are a group of molecules which undergo a ring closing and opening reaction under illumination with UV and visible light. They can retain their photochromic properties after binding to a silicon surface by a well-chosen linker molecule. Due to the large hyperpolarizability of the molecules the nonlinear optical (NLO) properties of the surface can be controlled by illumination with light. The samples were investigated with second harmonic generation (SHG), taking advantage of the symmetry of the substrate, which generates no SHG signal. We will show that a controlled photoinduced reversible change of the NLO properties of an indolylfulgimide functionalized silicon surface is possible.

CPP 56.11 Thu 17:45 S051

Reversible photo-switching of spiropyran molecules in direct contact with a single crystal — •Fabian Nickel, Matthias Bernien, Kai Kraffert, Dennis Krüger, Lucas M. Arruda, Lalminthang Kipgen, and Wolfgang Kuch — Institut für Experimentalphysik, Freie Universität Berlin, 14195 Berlin, Germany

The photochromic isomerization of molecules in direct contact with solid surfaces plays an important role for the further miniaturization of electronic devices. A good candidate for this purpose is spiropyran (SP). SP can be switched from a closed form to an open form (merocyanine, MC) by UV light and reversibly back by visible light. In nitro-spiropyran, however, the backreaction was found to be quenched on surfaces [1]. The modification of the end group from nitro- to naphtho-spiropyran leads to a lower electric dipole moment in the open form, which might favor switching back to the open form on a surface. In-situ x-ray absorption fine structure (NEXAFS) measurements at the nitrogen and oxygen edges prove and quantify the photoisomerization of these molecules on a Bi(111) surface. Illumination by UV light leads to an efficient switching to the open MC form of the molecule and, furthermore, a determination of the energy barriers of the photo-excited and metastable states becomes possible by temperature-dependent measurements. Visible light triggers the relaxation back to the closed SP form, thus offering full reversible control of the isomerization in direct contact with a single crystal surface.

This work is supported by the DFG through Sfb 658.

[1] Piantek et al. J. Am. Chem. Soc. 131, 12729 (2009).

CPP 57: Polymer Dynamics and Rheology (joint session CPP/DY, organized by CPP)

Time: Thursday 15:00–18:30 Location: H40

CPP 57.1 Thu 15:00 H40

Iso-flux tension propagation theory of driven polymer translocation through a nano-pore — •Jalal Sarabadani[1], Tapio Ala-Nissila[2], and Timo Ikonen[3] — [1]Department of Applied Physics, Aalto University, Espoo, Finland — [2]Department of Applied Physics, Aalto University, Espoo, Finland — [3]VTT Technical Research Centre of Finland Ltd., Espoo, Finland

We investigate the dynamics of pore-driven polymer translocation mainly by using analytical model and also by molecular dynamics (MD) simulations [1]. By using the tension propagation theory within the constant flux approximation an explicit equation of motion for the tension front is derived. This equation leads us to a scaling relation for the average translocation time, τ, which captures the asymptotic result $\tau \sim N_0^{1+\nu}$. Here, N_0 is the chain length and ν is the Flory exponent. Moreover, we derive the leading correction-to-scaling term to τ which is a finite chain length correction term ($\sim N_0$) due to the effective pore friction. Then by incorporating the fluctuations in the initial configuration of the polymer into the model in addition to thermal noise, the model not only reproduces previously known results but also considerably improves the estimates of the monomer waiting time distribution and the time evolution of the translocation coordinate $s(t)$, showing excellent agreement with MD simulations. We also discuss the effect of a flickering pore and an oscillating external driving force on the translocation time using the new model [2]. [1] J. Sarabadani, T. Ikonen and T. Ala-Nissila, J. Chem. Phys. (141), 214907 (2014). [2] J. Sarabadani, T. Ikonen and T. Ala-Nissila, J. Chem. Phys. (143), 074905 (2015).

CPP 57.2 Thu 15:15 H40

Polymer translocation through nanopores: An unbiased perspective on free energy landscapes and essential dynamics — Evangelos Tzaras, Florian Weik, Christian Holm, and •Jens Smiatek — Institut für Computerphysik, Universität Stuttgart, D-70569 Stuttgart, Germany

We studied the translocation of uncharged polymers through thin nanopores by coarse-grained Molecular Dynamics simulations in combination with a forward flux sampling approach. Our results for short and intermediate chain lengths reveal that the translocation behavior is mostly governed by the transition probabilities of single monomers. Specific configurational changes of the polymer or chain tension effects are minor important. We propose an analytic approach for the free energy landscapes which is in good agreement with the simulation results. The outcomes of an essential dynamics analysis verify that only a small number of eigenvectors is substantial for a reliable description of the polymer motion. A comparison with polymers in dilute bulk solution indicates the presence of quasi-equilibrium states which are important for the validity of the underlying free energy landscapes.

CPP 57.3 Thu 15:30 H40

The Origin of Strong Slip Of Polymer Melts on Structured Surfaces: A Molecular Approach. — •Mischa Klos[1], Laurent Joly[2], Sebastian Backes[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

Flow dynamics at the solid/liquid interface gain more importance when it comes to small scales. In special systems, a liquid can reach a finite velocity at the boundary to the solid. Our experiments probe this phenomenon via the dewetting of thin polymer films on hydrophobic substrates [1]. As hydrophobic coatings we use thin amorphous polymers films or different types of ordered self-assembled silane monolayers on silicon substrates. On silane surfaces, polystyrene (PS) of low molecular weight exhibit slip lengths up to micrometers [2]. On AF1600, no significant slip is observed. Scattering studies indicate an interfacial layer at the interface depending on the structure of the substrate [3]. Simulations where able to refine the molecular idea of the used SAMs [4]. However, strong slip is reduced if PMMA or polyvinylpyridine (PVP) are used instead of PS. MD-Simulations of our systems allow detailed insights into the dynamics of the polymer melt. [1] O. Bäumchen, et.al., J. Phys. Condens. Matter 24 325102 (2012) [2] R. Fetzer, et. Al., Europhys Lett. 75 638 (2006) [3] P. Gutfreund, et. al., Phys. Rev. E 87 012306 (2013) [4] J.M. Castillo Sanchez, et.al., Langmuir 31, 2630 (2015)

CPP 57.4 Thu 15:45 H40

Contact Kinetics in Fractal Macromolecules — •Maxim Dolgushev[1], Thomas Guérin[2], Alexander Blumen[1], Olivier Bénichou[3], and Raphaël Voituriez[3] — [1]Physikalisches Institut, Universität Freiburg, Hermann-Herder-Strasse 3, 79104 Freiburg, Germany — [2]Université de Bordeaux and CNRS, Laboratoire Ondes et Matière d'Aquitaine (LOMA), UMR 5798, 33400 Talence, France — [3]Laboratoire de Physique Théorique de la Matière Condensée, CNRS/UPMC, 4 Place Jussieu, 75005 Paris, France

We investigate the effect of the complex connectivity of macromolecules on the contact kinetics by focusing on the case of fractal macromolecules [1]. In our theoretical description, the non-Markovian feature of monomer motion, arising from the interactions with the other monomers, is captured by accounting for the non-equilibrium conformations of the macromolecule at the very instant of first contact. This analysis reveals a scaling relation for the Mean First Contact Time as a function of the equilibrium distance between the reactive monomers and of the spectral dimension of the macromolecule, which is independent on the microscopic details of the macromolecules. We show that the non-Markovian effects increase for the structures with higher degree of hyperbranching, for which the conformations at first contact are getting much more different from equilibrium looping conformations. Our theoretical predictions are in excellent agreement with numerical stochastic simulations.

[1] M. Dolgushev, T. Guérin, A. Blumen, O. Bénichou, and R. Voituriez, Phys. Rev. Lett. 115, 208301 (2015).

CPP 57.5 Thu 16:00 H40

Branch Point Motion in Asymmetric Star Polymers Investigated by Molecular Dynamics Simulations — •Stefan Holler[1,2], Angel Moreno[2], Michaela Zamponi[1], and Dieter Richter[1] — [1]Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Centro de Fisica de Materiales, 20018 San Sebastian, Spain

Large-scale molecular dynamics simulations of three-arm asymmetric star polymers have been performed to study the motion of the branch point and the so-called hopping parameter p^2 that characterizes the effective friction associated to the short side arm. The simulated star polymer systems consist of a large backbone (10 or 16 entanglements) and a central short unentangled side arm.

This work expands the investigation by Bacova et al. [1] in similar stars with entangled side arms. Surprisingly, the frictional contribution of the unentangled side arms on the motion of the linear backbone is much larger than assumed by theory. The value of p^2 can be calculated from the simulation data using general assumptions that hold true for all versions of hierarchical relaxation models. The most consistent description of the simulation results suggests that p^2 is not a constant but depends on architecture and molecular weight, and that hopping occurs in the bare, undilated tube.

[1] Bacova et al., Macromolecules 47 (2014) 3362

CPP 57.6 Thu 16:15 H40

Disentanglement of Two Overlapping Polymer Chains: Contacts vs. Knots — •Diddo Diddens, Nam-Kyung Lee, Sergei Obukhov, Jörg Baschnagel, and Albert Johner — Institut Charles Sadron, Université de Strasbourg, CNRS UPR22, 23 Rue du Loess, 67034 Strasbourg Cedex 2, France

The role of topological constraints is one of the remaining challenges in polymer physics. While it is evident that the non-crossability heavily affects the motion of long polymer chains in dense solutions and melts, these constraints are usually neglected in theoretical descriptions of the polymer dynamics in dilute solutions. However, the situation becomes less clear in the limit of long chains and/or rather dense polymer coils (e. g. close to the Θ-point), since even for a single chain, distinct segments are more likely to be intertwined or knotted.

To address this issue, we present a comprehensive study comprising MC and MD simulations as well as analytical calculations, and investigate the relevance of non-crossing constraints for two polymer chains brought into initial overlap. In particular, we join two long polymers by a labile bond, and focus on their separation directly after the cleavage of this bond. We demonstrate that the average time for this process strongly correlates with the number of monomeric contacts between the two strands. Moreover, in case of highly entangled or knotted starting configurations, the segregation time is several orders of magnitude larger than expected for a purely diffusive process, thus clearly highlighting the importance of topological constraints. Finally, we also give a brief account on the role of hydrodynamics.

15 min. break

CPP 57.7 Thu 16:45 H40

Static and dynamic properties of polymer melts: equilibrium and non-equilibrium molecular dynamics studies — •Hsiao-Ping Hsu and Kurt Kremer — Max Planck Institute for Polymer Research

We present a detailed study of the static and dynamic behavior of semiflexible polymer chains in a melt starting from the previously obtained fully equilibrated high molecular weight polymer melts by a hierarchical strategy. For semiflexible chains in a melt, we see that results of the mean square internal distance, the probability distributions of the end-to-end distance, and the chain structure factor are all described very well by the theoretical predictions for ideal chains to some extent. We examine the motion of monomers in polymer melts by molecular dynamic (MD) simulations using the ESPResSo++ package. The scaling predictions of the mean square displacement of monomers based on the Rouse model, and the reptation theory are verified, and the related characteristic relaxation time scales are determined. We also check the topological structures of polymer chains through the primitive path analysis (PPA), and give the evidence that the entanglement length determined through PPA in the standard expression of the plateau modules is consistent with the value obtained from stresses using the Green-Kubo relation. Finally, the non-linear viscoelastic properties of deformed polymer melts after a step uniaxial elongation and the conformational changes of chains during the relaxation process are investigated through a non-equilibrium MD study. We acknowledge the cooperation of G. Zhang, T. Stuehn, and K. Ch. Daoulas.

CPP 57.8 Thu 17:00 H40

Knots as Topological Order Parameter for Semiflexible Polymers — •Martin Marenz and Wolfhad Janke — Institut für theoretische Physik, Leipzig, Germany

We used a combination of the multicanonical Monte Carlo algorithm and the replica-exchange method to investigate the phase diagram of a semiflexible polymer in dependence of the polymer stiffness. We found a novel phase in the phase diagram which is best described by the knot type of the polymer conformation. Almost all conformations in these phases have the same knot type after applying a procedure which connects the termini of the polymer. Therefore, they are thermodynamically stable and considerable different from the knots found in the swollen and globular phase of flexible polymers. We also showed that a derivative of the Alexander polynomial is a well suited order parameter to distinguish the *knotted* phases. Moreover, the transitions into the knotted conformations exhibit a phase coexistence, but happen at an almost constant mean total energy, hence we observed no latent heat.

CPP 57.9 Thu 17:15 H40

Packing Length Dependence of Chain Dynamics in Polymer Melts near the Unentangled-Entangled Crossover — •Herwin Jerome Unidad[1], Michaela Zamponi[1], Oxana Ivanova[1], Lutz Willner[2], Wim Pyckhout-Hintzen[2], Andreas Wischnewski[2], Dieter Richter[2], and Lewis J Fetters[3] — [1]JCNS, Outstation at MLZ, Forschungszentrum Juelich, Garching, Germany — [2]JCNS-1/ICS-1, Forschungszentrum Juelich, Juelich, Germany — [3]Department of Chemical and Biological Engineering, Cornell University, Ithaca, New York

Recently, we showed that the ratio between the critical molecular weight (Mc) and the entanglement molecular weight (Me) does not have the universal value of 2 for all polymer melts but rather shows a subtle dependence on the so-called packing length (p). All three parameters are important in describing the rheology and chain dynamics of polymer melts. With this, the packing length seems to be an important length scale for describing the non-universality of chain dynamics. To clarify this role, we performed neutron spin echo experiments on two polymer series with various molecular weights and different packing lengths. We obtained a good description of the measured intermediate scattering function using the Rouse model by suppressing long-wavelength internal modes. We then examine how this mode suppression could proceed as a function of both the chain length and the packing length. These findings are explained in the framework of earlier ideas on entanglement formation.

CPP 57.10 Thu 17:30 H40

Disentanglement of polymers under shear — Maciej Kawecki[1], Philipp Gutfreund[2], Franz Adlmann[1], Stephane Longeville[3], Alain Lapp[3], Piotr Zolnieczuk[4], Peter Falus[2], and •Max Wolff[1] — [1]Department for Physics and Astronomy, Uppsala University, Sweden — [2]Institut Laue-Langevin, Grenoble, France — [3]Institut Leon Brillouin, Scala, France — [4]Oak Ridge National Laboratory, Oak Ridge, USA

Neutron Spin Echo spectroscopy provides unique insight into molecular and sub-molecular dynamics in soft matter. In polymer physics a stress plateau is observed for increasing shear rate, which might be explained by an entanglement-disentanglement transition and change the dynamics of the chains drastically. Neutron Spin Echo provides information about entanglement length and degree by probing the local dynamics of the polymer chains. Combining shear experiments and neutron spin echo is challenging since, first the beam polarisation has to be preserved during scattering and second, Doppler scattered neutrons may cause inelastic scattering. We demonstrate that a high beam polarisation can be preserved and present SANS data revealing shear-induced conformational changes in highly entangled polymers as well as Spin Echo measurements indicating an disentanglement transition under shear.

CPP 57.11 Thu 17:45 H40

Extensional and shear rheology as a powerful tool for characterisation of physical networks in polymer nanocomposites — •Milan Kracalik — Johannes Kepler University Linz, Institute of Polymer Science, Altenberger Str. 69, 4040 Linz, Austria

Polymer nanocomposites are an interesting class of materials, in particular in the field of light weight construction. With increasing knowledge about proper processing protocol and resulting nanocomposite structure and property profile, respectively, it is possible to utilize polymer nanocomposites in many applications like automotive or aerospace industry. During material development procedure, rheological investigation possesses crucial information about material structure/performance already in the processing stage. Therefore, right compilation and interpretation of rheological measurements can significantly speed up the developing procedure. In this contribution, selected polymer nanocomposites have been characterized by both extensional as well as shear rheology. Using novel evaluation of oscillatory shear flow data, it was possible to correlate data of shear rheometry with those of elongational rheometry and, consequently, to obtain complex rheological information about different physical networks of nanopartikel in polymer matrix.

CPP 57.12 Thu 18:00 H40

Co-non-solvency of smart polymers: Physical concepts and computer simulations — •Debashish Mukherji and Kurt Kremer — Max-Planck-Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Smart polymers are a modern class of soft materials that show drastic changes in their physical properties by a slight change in external stimuli. One such phenomenon is known as co-non-solvency. Co-non-solvency occurs when a polymer is added to a mixture of two (perfectly) miscible and competing good solvents. As a result, the same polymer collapses into a globule within intermediate mixing ratios. More interestingly, polymer collapses when the solvent quality remains good or even gets increasingly better by the addition of the better cosolvent [1]. This puzzling phenomenon, where the solvent quality is completely decoupled from the polymer conformation, is driven by strong local preferential adsorption of better cosolvent with the polymer [1,2]. Because a polymer collapses in good solvent, the depletion forces, that are responsible for poor solvent collapse, do not play any role in describing co-non-solvency [3]. Furthermore, it will be presented that this phenomenon can be understood within a universal (generic) concept. Therefore, a broad range of polymers is expected to exhibit co-non-solvency and the specific chemical details do not play any role in understanding these complex conformational behaviors [4].

[1] D. Mukherji and K. Kremer, Macromolecules (2013). [2] D. Mukherji, et al. Nat. Commun. (2014). [3] T. E. de Oliviera, et al., Soft Matter (2015). [4] D. Mukherji, et al, JCP (2015).

CPP 57.13 Thu 18:15 H40

PNIPAM dynamics in water-methanol mixtures — •Konstantinos N. Raftopoulos[1], Konstantinos Kyriakos[1], Olaf Holderer[2], Oxana Ivanova[2], Michael Ohl[3], Peter Müller-Buschbaum[1], and Christine Papadakis[1] — [1]Physik-Department, Technische Universität München, Garching, Germany — [2]JCNS at Outstation MLZ, Garching, Germany — [3]JCNS at Outstation Oak Ridge, Tennessee, USA

In aqueous solutions, at low temperatures, the hydrophilic groups of Poly(N-isopropylacrylamide) form H-bonds with the water molecules and the polymer dissolves. Above the cloud point, the chain dehydrates and phase-separates. Although the polymer dissolves well in methanol too, the cloud point in water-methanol mixtures decreases considerably with respect to that in aqueous solutions. The phenomenon is termed cononsolvency. The physical mechanisms behind the process are still not clear and even less is known about the dynamics. Aiming to shed some light in this question, we followed the segmental dynamics of the polymer in water-methanol mixtures by neutron spin echo spectroscopy. The experiments were performed 2 and 5 K below the cloud points, in a temperature region where the solution is in θ-conditions. Methanol slows down the segmental dynamics of the polymer, but there is no evidence for a change of the mobility mechanism. The deceleration is more pronounced at higher polymer concentrations.

CPP 58: Wetting, Nano- and Microfluidics II (joint session CPP/DY, organized by CPP)

Time: Thursday 15:00–16:45 Location: H42

CPP 58.1 Thu 15:00 H42

How water advances on superhydrophobic surfaces — •Frank Schellenberger, Noemí Encinas, Doris Vollmer, and Hans-Jürgen Butt — 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.

CPP 58.2 Thu 15:15 H42

Traction forces of water droplets on super-hydrophobic surfaces — •Martin Tress, Alexander Saal, Frank Schellenberger, and Noemí Encinas — Max Planck Institute for Polymer Research, Mainz

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 drop will be illuminated.

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

CPP 58.3 Thu 15:30 H42

Bioinspired Nanofur as Superhydrophobic Transparent Coatings and Translucent Films for Optical Applications — •Felix Vüllers, Maryna Kavalenka, Matthias Worgull, and Hendrik Hölscher — Institute of Microstructure Technology, Karlsruhe Institute of Technology, 76344 Karslruhe, Germany

A combination of high optical transmission with self-cleaning, water-repellency and anti-icing is of high interest for various optical applications and boosted interest to transparent superhydrophobic surfaces. We demonstrate a highly scalable hot-pulling method to produce flexible superhydrophobic thin nanofur films made from polycarbonate, which can be used both as a transparent coating and a translucent film. The surface of thin nanofur films is covered with densely packed high aspect ratio nano- and microhairs which are fabricated using heated sandblasted steel plates, making complex and expensive mold fabrication unnecessary. The films exhibit high water contact angles ($>170°$), low sliding angles ($<4°$) and self-cleaning abilities. Through index matching the thin nanofur coating's reflection in the visible regime is reduced to less than 4%. The translucent film's transmission is more than 85% with high forward scattering. Applied to OLEDs these optical properties lead to an efficiency increase of more than 10%. By combining these exceptional optical properties with the water-repellent and self-cleaning properties of the thin nanofur film, the films are beneficial for further optical devices. In addition plasma treatment changes the film wettability to underwater superoleophobic enabling the use of thin nanofur films as underwater oil-repelling coatings.

CPP 58.4 Thu 15:45 H42

Dynamics of Drop Condensation on Lubricant-Impregnated Surfaces — •Tadashi Kajiya[1], Frank Schellenberger[1], Periklis Papadopoulos[2], Doris Vollmer[1], and Hans-Jürgen Butt[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]University of Ioannina, Dept. of Physics, 45110 Ioannina, Greece

We explored the dynamics of water drops condensing on a lubricant-impregnated surface, i.e., micropillar arrays infused with a ionic liquid. Growing drops were imaged in 3D using a laser scanning confocal microscope equipped with a temperature and humidity control. On a lubricant-impregnated hydrophobic micropillar array, different stages of condensation can be discriminated: - Nucleation on a lubricant surface. - Regular alignement between micropillars and formation of a three-phase contact line on a bottom of the substrate. - Deformation and bridging by coalescence, leading to a detachment of the drops from the bottom substrate to pillars*top faces. However, on a lubricant-impregnated hydrophilic micropillar array, the condensed water covers the micropillars by dewetting the lubricant. As a result, the surface loses its slippery property. Our results provide fundamental concepts how these solid/liquid hybrid surfaces can be applied for facile removal of condensed water.

CPP 58.5 Thu 16:00 H42

Connecting and disconnecting nematic disclination lines in microfluidic channels — •Hakam Agha and Christian Bahr — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Fassberg 17, 37077 Göttingen, Germany

The controlled creation of a disclination line in nematic liquid crystal (NLC) spanning along the microfluidic channel as a result of imposed anchoring conditions on the four confining channel walls has proven to be a novel and successful approach to guided transport of microfluidic cargo, with the disclination line serving as a soft rail [1]. In this study, we report on a method to connect and disconnect disclination lines using the interplay between anchoring, flow, and electric field. We design the anchoring conditions in a way that the formation of the disclination is suppressed in one or several short sections of the channel. The application of an external electric field across the channel and perpendicular to the NLC flow can overcome the imposed anchoring conditions and allows the disclination line to span across the forbidden regions, establishing a continuous disclination along the complete channel. Thus, the manipulation of the anchoring conditions combined with the effect of the electric field allows us to interrupt and to reestablish the transport of colloidal particles through the microchannel.

[1] A. Sengupta, C. Bahr, S. Herminghaus, Soft Matter, 2013, 9, 7251.

CPP 58.6 Thu 16:15 H42

Lateral Adhesion Forces at Solid-Liquid Interfaces — •Nan Gao, Florian Geyer, Sanghyuk Wooh, Dominik Pilat, Doris Vollmer, Hans-Jürgen Butt, and Rüdiger Berger — Max Planck Institute for Polymer Research, Mainz, Germany

Using a laser deflection system we investigate lateral adhesion forces at solid-liquid interfaces. Our set-up consists of a laser, a deflectable capillary, and a position sensitive detector (PSD). Substrates of TiO2 nanopillars with various spacing distances between the nanopillars are used to regulate surface wettabilities. Drops of liquid resting on the nanopillar substrates have different lateral adhesion forces due to the surface wettabilities. In order to measure the forces at the solid-liquid interfaces, the drops are moved laterally against the substrates using the deflectable capillary. A laser beam incident on the capillary is reflected to the PSD, which instantly generates electric signals according to the lateral adhesion forces. With assistance of optical imaging, we have been able to resolve the drop motion synchronised to the force measurement. Our measurements have demonstrated that the instantaneous lateral adhesion forces at the solid-liquid interfaces are determined by the front and rear contact angles as well as the contact width. The values are in good agreement with theoretical predictions.

CPP 58.7 Thu 16:30 H42

Light-driven delivery and release of materials using liquid marbles — •Maxime Paven[1], Hiroyuki Mayama[2], Takafumi Sekido[3], Hans-Jürgen Butt[1], Yoshinobu Nakamura[3,4,5], and Syuji Fujii[4] — [1]1Physics at Interfaces MaxPlanck Institute for Polymer Research Ackermannweg 10, D-55128 Mainz, Germany — [2]2Department of Chemistry, Asahikawa Medical University 2-1-1-1 Midorigaoka-Higashi, Asahikawa 078-8510, Japan — [3]3Division of Applied Chemistry, Graduate School of Engineering Osaka Institute of Technology 5-16-1 Omiya, Asahi-ku, Osaka, 535-8585, Japan. — [4]4Department of Applied Chemistry, Faculty of Engineering, Osaka Institute of Technology 5-16-1 Omiya, Asahi-ku, Osaka, 535-8585, Japan. — [5]5Nanomaterials Microdevices Research Center Osaka Institute of Technology 5-16-1 Omiya, Asahi-ku, Osaka 535-8585, Japan.

Remote control of the locomotion of small objects is a challenge in itself and may also allow for the stimuli control of entire systems. Here, we describe how encapsulated liquids, referred to as liquid marbles, can be moved on a water surface with a simple near-infrared (NIR) laser or sunlight. Using light rather than pH or temperature as an external stimulus allows for the control of the position, area, timing, direction and velocity of delivery. Our approach makes it possible to not only transport the materials encapsulated within the liquid marble but also to release them at a specific place and time, as controlled by external stimuli. Furthermore, we show that liquid marbles can work as light-driven towing engines to push or pull objects.

CPP 59: Biomaterials and Biopolymers III (joint session BP/CPP/MM, organized by BP)

Joint session with CPP and MM organized by BP.

Time: Thursday 15:00–16:15 Location: H45

CPP 59.1 Thu 15:00 H45

Contribution of Biofilm Matrix Components to Physical Material Properties of Bacterial Biofilms — •Sara Kesel, Stefan Grumbein, Ina Gümperlein, Anna-Kristina Marel, Marwa Tallawi, Oliver Lieleg, and Madeleine Opitz — Center for NanoScience, Faculty of Physics, Ludwig-Maximilians-Universität München, Munich, Germany

Bacteria can be protected from antibiotics, chemicals and mechanical stresses by a self-produced matrix, the so called biofilm. As biofilms can grow on various surfaces such as medical implants, this poses a big problem in health care and industry. Biofilm matrices can thereby consist of different extracellular substances (EPS) such as polysaccharides, proteins, lipids and nucleic acid. Understanding of the individual contributions to the above described resistances by the different biofilm matrix components is therefore necessary, in order to prevent and fight biofilm growth. In particular, it is important to understand at what stage of biofilm formation the observed resistances are developed. In this study, different stages of biofilm growth (attachment of single cells, microcolony growth, as well as mature biofilms) were investigated using several techniques such as e.g. cantilever arrays, time-lapse microscopy and atomic force microscopy. The attachment of single bacteria onto solid surfaces and further physical material properties of two B. subtilis wild-type strains that differ in their biofilm matrix composition were analyzed. Furthermore, using several mutant strains the impact of specific biofilm matrix elements on the observed biofilm properties was quantitatively analyzed.

CPP 59.2 Thu 15:15 H45

Multiple bio-functionalization in 3D-scaffolds for cell manipulation realized by orthogonal (photo)chemistry — •Vincent Hahn[1], Benjamin Richter[2], Tanja Claus[3,4], Guillaume Delaittre[3,5], Christopher Barner-Kowollik[3,4], Martin Wegener[1,6], and Martin Bastmeyer[2] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT) — [2]Zoological Institute and Institute for Functional Interfaces, KIT — [3]Institute for Chemical Technology and Polymer Chemistry, KIT — [4]Institute for Biological Interfaces, KIT — [5]Institute for Toxicology and Genetics, KIT — [6]Institute of Nanotechnology, KIT

In recent years, we have applied Direct Laser Writing to fabricate 3D-microscaffolds for culturing cells in a well-defined environment and investigated cellular responses, e.g., contractility, adhesion and shape.

By sequential writing of different photoresists, patterned scaffolds are realized. They consist of protein-binding polymers next to regions containing light-activatable monomers in a non-protein binding background. Upon light-activation we were able to biotinylate specific regions in the passivating backbone. When incubated with a protein solution, proteins adsorb only onto protein-binding polymer areas. The biotin-linker is subsequently addressed by using avidin and any other biotinylated protein of choice. This technique has been successfully applied to fabricate scaffolds functionalized with two different adhesion proteins that selectively direct cell adhesion.

Such scaffolds might prove useful for applications in tissue engineering and stem cell differentiation.

CPP 59.3 Thu 15:30 H45

Different protein adsorption rates on different grain orientations in hydroxyapatite — •Thomas Faidt, Jörg Schmauch, Michael Deckarm, Samuel Grandthyll, Frank Müller, and Karin Jacobs — Saarland University, Dept. of Experimental Physics, 66041 Saarbruecken

As a model system for tooth enamel, hydroxyapatite (HAP) pellets with a density of $> 97\%$ of the theoretical crystallographic density of HAP have been produced by compacting and sintering commercially available HAP powder. Atomic force microscopy (AFM) combined with electron backscatter diffraction (EBSD) measurements reveal the smoothness and the crystal orientation of the HAP grains on the surface of the pellets. On these surfaces, single molecule BSA adsorption experiments are performed in a microfluidic setup and reveal that different grain orientations provoke different adsorption rates. These findings open a pathway to control protein adsorption.

CPP 59.4 Thu 15:45 H45

Studying Biomineralization with ultrathin silica sheets grown at the air-water interface. — •Helmut Lutz[1], Vance Jaeger[2], Rüdiger Berger[1], Mischa Bonn[1], Jim Pfaendtner[2], and Tobias Weidner[1] — [1]Max Planck Institute for Polymer Research Ackermannweg 10, Mainz 55128, Germany — [2]Chemical Engineering University of Washington 105 Benson Hall, Seattle, WA 98195-1750, USA

Inspired by diatom silification we used amphiphilic peptides consisting of leucine and lysine (LK peptides) to investigate biomineralization at surfaces. Depending on hydrophobic periodicity, these peptides adopt alpha helical or beta sheet structures at the air-water interface. Upon addition of a silica precursor we obtained surface-tailored peptide-silica hybrid films with a thickness of ~4 nm. We probed film composition and interactions between peptides and silica at early stages of biomineralization by means of surface sensitive techniques, such as sum frequency generation (SFG) and X-ray photoelectron spectroscopy (XPS). Electron and atomic force microscopy show similarities of the film fine structure and the surface of in-solution silica precipitates. Experimental findings were complemented with molecular dynamics simulations. We believe that our results provide insights into the biomineralization of structured films, which might prove useful in materials design and surface engineering.

H. Lutz, V. Jaeger, R. Berger, M. Bonn, J. Pfaendtner, T. Weidner, Advanced Materials Interfaces 2015, 2, n/a. J. E. Baio, A. Zane, V. Jaeger, A. M. Roehrich, H. Lutz, J. Pfaendtner, G. P. Drobny, T. Weidner, Journal of the American Chemical Society 2014, 136, 15134.

CPP 59.5 Thu 16:00 H45

AFM force spectroscopy with S. aureus and Strep. mutans to reveal biopolymer binding properties — •Friederike Nolle[1], Nicolas Thewes[1], Christian Spengler[1], Kordula Schellnhuber[1], Peter Loskill[1], Alexander Thewes[2], Ludger Santen[2], and Karin Jacobs[1] — [1]Saarland University, Dept. of Experimental Physics, 66041 Saarbruecken — [2]Saarland University, Dept. of Theoretical Physics, 66041 Saarbruecken

The adhesion of pathogenic bacteria is a crucial step in the development of implant-related infections. The adhesion of bacteria is mediated by biopolymers, the properties of which we are able to characterize by AFM force spectroscopy, where the probe is a single bacterium. To deepen the understanding, we combine the AFM studies with computer simulations [1]. For bacteria (Staphylococcus aureus) in contact with hydrophobic surfaces, thermally fluctuating cell wall proteins of different stiffness attach to the surface via short range forces and subsequently * due to entropic forces * pull the bacterial cell into close contact. That way, S. aureus is able to substantially increase its interaction range for contact initiation. Bacteria like Streptococcus mutans also attach to hydrophilic surfaces (e.g. titanium or hydroxyapatite) in the presence or absence of other biomolecules (proteins, enzymes). Our study reveals the importance of specific parameters (e.g. roughness) and proposes that fluctuations in protein density and structure are much more relevant than the exact form of the binding potential.

[1] N. Thewes, P. Loskill, P. Jung, H. Peisker, M. Bischoff, M. Herrmann, K. Jacobs, Soft Matter 2015, 11, 8913-8919

CPP 60: Focus: Two Dimensional Functional Materials II

Time: Thursday 15:00–16:00 Location: H51

Invited Talk CPP 60.1 Thu 15:00 H51

Evolution of mono- and bilayer graphene in chemical vapor deposition and the thinnest feasible porous membranes for ultimate mass transport — •Hyung Gyu Park — Nanoscience for Energy Technology and Sustainability, Department of Mechanical and Process Engineering, ETH Zurich, Zurich, Switzerland

Graphene as the seminary 2D material poses great potential in many applications for its electronic, thermal, optical and mechanical properties unique and superior to other materials. Today a majority of technological applications use graphene produced via chemical vapor deposition and transferred onto destination substrates. This talk will present overview and our results of the growth of mono- and bilayer graphene on copper foils, leading to a discussion on kinetics, energetics and mechanisms of the graphene formation on copper. An interesting demonstration of the thinnest feasible porous membranes by use of our graphene illustrates the promises that 2D materials pose. Gas transport across the 2D porous membrane shows a wide range of transport mechanisms from free molecular to transition to continuum dynamics. Water transport measurement agrees well with a capillarity effect and an orifice theory. Discussion on technological implications will follow.

CPP 60.2 Thu 15:30 H51

Cluster Formation of Carbon Nanotubes in Lipid Bilayers — •Martin Vögele, Jürgen Köfinger, and Gerhard Hummer — Max-Planck-Institut für Biophysik, Frankfurt am Main

We investigate the clustering behavior of open-ended carbon nanotubes in lipid membranes by means of atomistic and coarse-grained molecular dynamics simulations. On the atomistic scale, we gain insight in the interactions of the nanotubes with lipids and with each other. The coarse-grained scale allows us to simulate the clustering of one hundred nanotubes for tens of microseconds. In our simulations, we vary parameters such as tube length and tube diameter. We also consider different functionalization of the carbon nanotubes, as well as different lipid compositions of the membrane.

We find that the up-right carbon nanotubes induce strong order in the lipids, which form ring-like structures around the tubes. Nanotubes quickly form clusters in which neighboring nanotubes are separated by a single layer of lipids, although free energy calculations suggest that direct nanotube contacts are more favorable. Only when we reduce lipid-nanotube interactions significantly, we observe the spontaneous formation of direct contacts. Thus, depending on the lipid-nanotube interactions, clusters can be kinetically trapped, which has important implication for large-scale applications.

CPP 60.3 Thu 15:45 H51

Graphitic carbon nitrides as graphene complements: new insights and challenges — •Christoph Merschjann — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin

"Graphitic" carbon nitride (CN) polymers are currently studied all over the world, mainly for photocatalytic processes like metal-free solar water-splitting, but also for solid-state lighting, hybrid photovoltaics, and organic electronics in general. Bearing its name due to a two-dimensional polymeric structure, the CN material class shows several fascinating properties, such as tunable optical band gap in the UV-VIS-IR range, comparably easy synthesis processes, and high chemical and thermal stability.

Just recently we could deduce the charge carrier mobility from transient fluorescence measurements, showing that the CN material class comprises reasonable candidates for optoelectronic applications. Moreover, we found that charge transport is mainly confined to channels perpendicular to the two-dimensional structure [1]. The materials thus complement graphene, possibly opening the way for novel applications.

The talk will give an overview of the latest opto-electronic physical findings in different CN materials as well as a discussion of the challenges of such measurements in optically scattering samples.

[1] C. Merschjann et al., *Advanced Materials* **2015**, DOI: 10.1002/adma.201503448

CPP 61: Interfaces and Thin Films I (joint session CPP/DY, organized by CPP)

Time: Thursday 16:15–18:15 Location: H51

Invited Talk CPP 61.1 Thu 16:15 H51

Tuning of ordering in colloidal suspensions confined in thin films — Sebastian Schön[1], Yan Zeng[1], Sabine Klapp[2], and •Regine von Klitzing[1] — [1]TU Berlin, Institut für Chemie, Strasse des 17. Juni 124, 10623 Berlin — [2]TU Berlin, Institut für Theoretische Physik, Hardenbergstraße 36, 10623 Berlin

Characteristic lengths of the structuring of silica nanoparticle suspensions confined between two silica surfaces were extracted from the oscillatory force profile of colloidal-probe atomic force microscopy (CP-AFM) measurements and compared with the bulk counterparts as obtained from structural peak of small angle X-ray scattering (SAXS). The wavelength λ extracted from CP-AFM correlates well with the mean particle distance 2π/qmax as obtained from SAXS structural peak. This observation suggests that there is no confinement effect on characteristic lengths themselves that represent the structuring, even though the confinement indeed induces a layered structure of the particles. A more quantitative study shows a relation of oscillatory wavelength of silica nanoparticle suspensions with the particle number density as λ=ρ-1/3, irrespective of particle size, surface charge of the particles and ionic strength of the solution. CP-AFM measurements on modified and deformable confining surfaces show an increase in amplitude with increasing surface potential and decreasing surface roughness and deformability. However, the corresponding wavelength remains unaffected. Current studies address the ordering of soft particles like thermosensitive nanogels in the confinement of thin films, where the inter particle interactions can be switched on and off.

CPP 61.2 Thu 16:45 H51

Highways for ions in polymers - 3D-imaging of electrochemical interphase formation — •Karl-Michael Weitzel[1], Veronika Wesp[1], Julia Zakel[1], Martin Schäfer[1], Ilka Paulus[2], and Andreas Greiner[2] — [1]Fachbereich Chemie, Philipps-Universität Marburg — [2]Makromolekulare Chemie II, Universität Bayreuth

The formation of a cesium interphase in-between a polymer film and a platinum electrode has been initiated by low energy bombardment induced ion transport [1]. To this end two different samples of a poly (p-xylylene)(PPX) film, deposited on a platinum electrode have been bombarded by a low energy cesium ion beam. Ions are transported through the film according to the laws of electro-diffusion. They are neutralized at the interface between the PPX film and the metal electrode. Consequently, a cesium interphase is formed. 3D imaging of the interphase by means of time-of-flight secondary ion mass spectrometry (ToF-SIMS) reveals a correlation between structural characteristics of the interphase and conduction properties of the PPX film. The bombardment of PPX films consisting of a homogenous network leads to the formation of a uniform interphase. The bombardment of PPX films with nonintermittent pathways (NIPs) for the transport of ions leads to the formation of cesium islands which ultimately spread out laterally leading to a non-uniform interphase behind the PPX film. This picture is supported by measurements of the ionic conductivity which differs characteristically for the two kinds of PPX films.

[1] Wesp et al., Electrochimica Acta, 170 (2015) 122-130

CPP 61.3 Thu 17:00 H51

Evidence of a three-Layered structure in ultra-thin PVME and PVME/PS blend Films by nano-sized relaxation spectroscopy — •Sherif Madkour[1], Paulina Szymoniak[1], Mojdeh Heidari[2], Regine von Klitzing[2], and Andreas Schönhals[1] — [1]BAM Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12205 Berlin (Germany) — [2]Technische Universität Berlin, Straße des 17. Juni 124, 10623 Berlin (Germany)

Despite the many controversial discussions about the nanometric confinement effect on the properties of ultrathin films, many details remain not understood and/or experimentally unproven. Here, a combination of Broadband Dielectric Spectroscopy (BDS), Specific Heat Spectroscopy (SHS), and ellipsometry was utilized to investigate the glassy dynamics of ultra-thin films of Poly (vinyl methyl ether) (PVME) and PVME/Polystyrene (PS) 50:50 wt-% miscible blend (thicknesses: 8nm - 200nm). For BDS measurements, a recently developed nanostructured sample arrangement; where ultra-thin films are spin-coated on an ultra-flat highly conductive silicon wafer and sandwiched between a wafer with nanostructured SiO2 nano-spacers, was used. For PVME films, two processes were observed and interpreted to be the α-processes of a bulk-like layer and an absorbed layer to the substrate. BDS and SHS showed that glassy dynamics are bulk-like. However, for films lower than 15nm, BDS showed weakly slowed dynamics. For PVME/PS blend, by measuring the dynamic Tg in dependence on the film thickness, both BDS and SHS, showed that the Tg of the whole film was strongly influenced by a nanometer thick surface layer.

CPP 61.4 Thu 17:15 H51

Molecular Structure of Polyelectrolyte/Surfactant Mixtures with Tunable Electrostatic Interactions at Air-Water Interfaces — •Felix Schulze-Zachau and Björn Braunschweig — Institute of Particle Technology (LFG), Friedrich-Alexander University of Erlangen-Nürnberg (FAU), Cauerstrasse 4, 91058 Erlangen, Germany

Mixtures of poly(sodium 4-styrenesulfonate) (NaPSS) polyelectrolytes and cetyltrimethylammonium bromide (CTAB) surfactants were studied at the air/water interface with tensiometry, ellipsometry and vibrational SFG spectroscopy. Additionally, macroscopic foams from these mixtures were studied in order to relate information on the interfacial molecular structure and charging state to foam stability and foamability. At low NaPSS concentrations, hydrophobic PSS$^-$/CTA$^+$ complexes adsorb at air/water interfaces with co-adsorbed free CTA$^+$ ions. The latter leads to relatively stable foams. For mixtures with equimolar concentrations, there is a significant rise in surface tension to values close to the tension of neat water that is accompanied by negligible foamabilities. However, SFG spectroscopy and ellipsometry provide evidence that PSS$^-$/CTA$^+$ complexes are at the interface with high coverage. Obviously, at these concentrations PSS$^-$/CTA$^+$ complexes are highly solvated at the interface but in a subsurface configuration with a covering water layer with free OH groups that give a clear signature in our SFG spectra. For excess NaPSS concentrations, surface adsorption is mainly determined by the molecular properties of PSS$^-$ interfacial layers which provide good foamability and stability.

CPP 61.5 Thu 17:30 H51

Structure of films prepared from block copolymer mixtures: computer simulations and GISAXS experiments — •Anatoly V. Berezkin[1], Justus Oberhausen[1], Florian Jung[1], Dorthe Posselt[2], and Christine M. Papadakis[1] — [1]Technische Universität München, Physik Department — [2]Roskilde University, Department of Science, Systems and Models, Denmark

Block copolymer films are promising as nano-structured templates, e.g. for lithography. Mixtures of block copolymers provide a robust route towards the preparation of non-trivial morphologies with an easily controlled domain size. We investigated a mixture of short and long symmetric diblock copolymers experimentally using GISAXS and in simulations (dissipative particle dynamics). We addressed the case, when macrophase separation of the mixture is expected along with the microphase separation in each of two phases. Simulations, in accordance with the experiment, show that the phase rich in short chains is usually located near the film surfaces, while long chains concentrate in the film core. Thick lamellae in the film core are usually perpendicular to the substrate, while thin lamellae in the interfacial layers can be parallel or perpendicular, depending on polymer/surface interactions. Selective adsorption of one block stabilizes lying lamellae. In very thin films confined between two selective surfaces, the conflict between orientations of thick standing lamellae and thin lying lamellae leads to unusual lens-like non-orthogonal structures.

CPP 61.6 Thu 17:45 H51

Adsorption Behavior of a rigid Polyelectrolyte/Surfactant Mixture at the Air/Liquid Interface and its Influence on Foam Film Stability — •Martin Uhlig[1], Andreas Wohlfarth[2], Klaus-Dieter Kreuer[2], and Regine v. Klitzing[1] — [1]Technische Universität Berlin — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart

The properties of foams are of interest for many industrial applications such as enhanced oil recovery and in personal care products and are therefore the subject of many studies. To control and manipulate the properties of a foam, it is essential to understand the behavior of the single building blocks, the so-called foam films. A way to produce stable foam films is to mix surfactants with oppositely charged polyelectrolytes, as highly surface-active complexes can be formed with the two compounds. Extensive research on such mixtures was already performed with the focus on very flexible Polyelectrolytes, as PSS and PAMPS. However, it is still unclear what the influence of the backbone rigidity of the polyelectrolyte on the resulting foam film properties is. In this work a mixture of a newly synthesized polyelectrolyte (S220) with a stiffer backbone is used and mixed with the catanionic surfactant C14TAB. The system has been investigated by means of surface tension measurements, surface elasticity, foam film stability measurements and neutron reflectometry. Those measurements have shown a much higher surface activity and foam stability for the S220/C14TAB mixture then for mixtures with more flexible polyelectrolytes.

CPP 61.7 Thu 18:00 H51

Excluded Volume Effects in Polymer Brushes at Moderate Chain Stretching — •Dirk Romeis and Michael Lang — Leibniz Institut für Polymerforschung Dresden e.V.

We develop a strong stretching approximation for a polymer brush made of self-avoiding polymer chains [1]. The density profile of the brush and the distribution of the end monomer positions in stretching direction are computed and compared with simulation data. We find that our approach leads to a clearly better approximation as compared to previous approaches based upon Gaussian elasticity at low grafting densities (moderate chain stretching), for which corrections due to finite extensibility can be ignored. In addition, we test our predictions for the obtained scaling form of the distribution of free chain ends. In contrast to the previous approaches our scaling form is confirmed by simulation data.

[1] Romeis, D.; Lang, M.; Journal of Chemical Physics **141** (10) 104902 (2014)

CPP 62: Organic Electronics and Photovoltaics III (joint session CPP/DS/HL/O, organized by CPP)

Time: Friday 9:30–12:00 Location: H40

CPP 62.1 Fri 9:30 H40

Influence of order and disorder on some photovoltaic properties of AnE-PV polymers - a DFT study — •Chuan-Ding Dong and Wichard J. D. Beenken — Institut für Physik und Institut für Micro- und Nanotschnologie, Technische Universität Ilmenau, Germany

Recently, the copolymer poly(p-anthraceneethynylene-alt-poly(p-phenylenevinylene) (AnE-PV) has turned out to be a promising model for the effect of order and disorder in polymer-based solar cells.[1] By substituting linear octyl or branched 2-ethyl-hexyl sidechains to the conjugated backbone, the structure of AnE-PV can be tuned from order to disorder. Using Grimme's correction for dispersion in our DFT calculations, we will show that the van-der-Waals interaction between the sidechains influences the planarity of the conjugated backbones significantly. Consequently, we found order-dependent shifts of the respective absorption spectra, which are in agreement with the experimental data. Furthermore, we will demonstrate the effect of the alternative sidechain substitution on the stacking of AnE-PV copolymers to semi-crystalline aggregates, which is crucial for the efficiency of polymer solar cells.

[1] Kästner, C.; Egbe, D.; Hoppe, H.: *J. Mater. Chem. A* **3**(2015)395.

CPP 62.2 Fri 9:45 H40

Influence of surface characteristics on electronic properties of polymer thin films — •Philipp Ehrenreich, Susanne Birkhold, Alexander Graf, Eugen Zimmermann, Hao Hu, Kwang-Dae Kim, and Lukas Schmidt-Mende — Department of Physics, University of Konstanz, POB M 680, Konstanz 78457, Germany

Many applications in polymer electronics demand not only for a loss-free charge percolation pathway towards electrodes, but also a highly delocalized pi-orbital system for efficient charge generation after exciton dissociation. The latter is especially important for the development of all-polymer solar cells, in order to compete with fullerene-based devices. Within this work the influence of surface characteristics on structural, or rather electronic properties of polymer thin films is investigated by means of an H/J-aggregate analysis on the model polymer Poly(3-hexylthiophene).

CPP 62.3 Fri 10:00 H40

Quantum Molecular Dynamical Calculations of Poly(3,4-ethylenedioxythiophene) and its derivatives — •Amina Mirsakiyeva, Håkan W. Hugosson, and Anna Delin — KTH Royal Institute of Technology, Department of Material and Nanophysics, SE-16440, Sweden

Organic thermoelectrics (TE) are materials with the ability to produce an electrical current from a temperature gradient (the so-called Seebeck effect) and the advantages of organic compounds, such as less toxicity. Organic TE are based on conductive polymers where the conjugation between double and single bonds creates the π-bonds overlapping and consequently allows charge carriers transport along the polymer backbone. Up to this date, the most studied organic TE material is poly(3,4-ethylenedioxythiophene) (PEDOT). Its transparency, high stability in the oxidized state and ability to form water-soluble polyelectrolytes bring it to the leading position in industry. The success of PEDOT makes also its selenium (PEDOS) and tellurium (PEDOTe) derivatives promising thermoelectric materials. Here, we present theoretical calculations of PEDOS and PEDOTe. We determined structures of the polymer chains of PEDOS and PEDOTe, investigated HOMO and LUMO and calculated point-charge distributions along the polymer backbone. Our analysis aims at finding the localization of a polaron, i.e. the electronic excitation resulting in localized structural changes and charge accumulation. Such a deeper atomistic understanding of the processes inside thermoelectric materials will hopefully allow an improvement of the thermoelectric qualities of conductive polymers.

CPP 62.4 Fri 10:15 H40

How Morphology Affects the Charge Transport: A Case Study for C60 — •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, Technische Universität Dresden, 01062 Dresden, Germany — [2]Dresden Center for Computational Materials Science, Technische Universität Dresden, 01062 Dresden, Germany — [3]Center for Advancing Electronics Dresden, Technische Universität Dresden, 01062 Dresden, Germany

The performance of organic electronic devices is significantly influenced by the morphology of the individual layers. However, theoretical studies can cover mostly only highly ordered or completely amorphous systems.

We present a computational algorithm for the construction of arbitrarily ordered films ranging from amorphous to polycrystalline and highly crystalline. We demonstrate its application for a systematic study of the electron mobility in C60 systems depending on the degree of ordering which is based on a full parameterization of the electronic properties. Additionally, we present a generalization for other molecular materials such as pentacene as well as organic blends.

CPP 62.5 Fri 10:30 H40

Intermolecular hopping transfer between DPP-based donor-acceptor polymers: A first principle study — •Florian Günther[1,2], Sibylle Gemming[1,3], and Gotthard Seifert[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institute of Physical Chemistry and Electrochemistry, Dresden University of Technology, Dresden, Germany — [3]Institute of Physics, Technical University Chemnitz, Germany

Diketopyrrolopyrrole (DPP) based materials have recently been considered as promising candidates for novel organic electronics. Here, we report about our investigation on intermolecular charge transfer between DPP-based polymers. We utilize Marcus transfer theory and evaluate the required quantities, the reorganisation energy and the coupling, by density functional-based tight binding (DFTB) calculations.. Due to its computational efficiency as well as the opportunity to tune some calculation features, the DFTB method is well suited for this purpose. In doing so, the coupling elements have been calculated for various stacking formations. In order to derive a single quantity, which can been used for calculate the transfer rates, an energy-weighted statistical approach has been utilised.

The obtained values allow to analyse the charge carrier mobilities in dependence of isomeric effects as the orientation of the individual units, of the molecular structure as fuctionalization, or the meaning of stacking properties as parallel and anti-parallel.

15 min. break

CPP 62.6 Fri 11:00 H40

Comparison of electrostatic, inductive and dispersive excitation energy shifts for the example of a molecular crystal — •Jörg Megow — University of Potsdam, Germany

The description of dispersive excitation energy shifts is necessary whenever different molecules within a supramolecular aggregate experience a different environment. A new approach that is based on an extended dipole approximation for higher transition densities in the sum over states expression [1] allowed for an appropriate description of gas-to-crystal-shifts in thin 3,4,9,10-perylenetetracarboxylic diimide (PTCDI) films [2]. It was also possible to explain the splitting of the main bands in the UV/Vis spectrum of double-walled tubular cyanine aggregates [3] as well as the line shift and broadening of the measured UV/Vis spectrum of pheophorbide *a* dendrimers [4]. For the example of a PTCDI crystal the different contributions to the overall site energy shifts are calculated while approximating the sum over states expressions for the energy shifts due to dispersion and inductive polarization, respectively. It is shown that the dispersive site energy shift dominates the site energy shifts due to electrostatic interaction and inductive polarization.

[1] A. Stone, *The theory of intermolecular forces*, Oxford University Press (2013); [2] J. Megow, T. Körzdörfer, T. Renger et al., J. Phys. Chem. C 119, 5747-5751 (2015); [3] J. Megow, M. I. S. Röhr, M. Schmidt am Busch et al., PCCP 17, 6741-6747 (2015); [4] J. Megow, ChemPhysChem 16, 3101-3107 (2015)

CPP 62.7 Fri 11:15 H40

Efficient first-principles based screening for high charge carrier mobility in organic crystals — •Christoph Schober, Karsten Reuter, and Harald Oberhofer — Technische Universität München

In organic electronics, charge carrier mobility is a key performance parameter. Due to the complex manufacturing processes of e.g. organic field effect transistors (OFETs) measured mobilities are often heavily affected by the device preparation. This masks the intrinsic materials properties and therewith hampers the decision whether further device optimization for a given organic molecule is worthwhile or not. We developed a fast and efficient protocol with a descriptor based on electronic coupling values to assess the expected performance of organic materials for application in organic electronic devices. Applying this protocol to experimental structures of organic crystals obtained from the Cambridge Structural Database (CSD), we screened about 40000 structures employing only first principle methods. Out of the 28000 successfully calculated structures we selected 2000 candidates with above- average electronic couplings for additional calculations and in-depth analysis using statistical methods and automated classification based on chemical structure. This allowed us not only to identify a number of specific crystals with exceptionally high electronic coupling values and therefore promising properties, but also possible lead structures which can be the basis for in-depth theoretical and experimental studies of new classes of materials for organic electronics.

CPP 62.8 Fri 11:30 H40

In-situ x-ray investigation of the structure formation of metal films on photoactive polymers — •Franziska C. Löhrer[1], Volker Körstgens[1], Matthias Schwartzkopf[2], Alexander Hinz[3], Oleksandr Polonskyi[3], Thomas Strunskus[3], Franz Faupel[3], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Deutsches Elektronensynchrotron DESY, 22607 Hamburg, Germany — [3]CAU zu Kiel, Institut für Materialwissenschaft, LS Materialverbunde, 24143 Kiel, Germany

Photoactive polymers have received high attention in recent years due to a large variety of different applications in molecular electronics. Although organic materials are used in the active layers of these devices, typically in many cases the electrodes are still made from metals. Thus, the polymer-metal interfaces are inherently present in all these novel devices. Our work takes a deeper look at the morphology of interfaces between photoactive layers and metal contacts deposited on top of them. We investigate morphological changes during sputter deposition of metal films (electrodes) onto photoactive films using in-situ GISAXS. Probing the sputter process in-situ allows highly time resolved insights into the deposition behavior of the metal depending on the polymer layer's properties. The deposition behaviors of gold and aluminium are compared, as both metals are frequently used as electrodes. The photoactive films consist of the low band gap polymer PTB7 as well as of PTB7:PCBM blends. The final film morphology is characterized via SEM and XRR after sputter deposition.

CPP 62.9 Fri 11:45 H40

Charge-Transfer - Solvent Interaction Predefines Doping Efficiency in p-Doped P3HT-Films — •Lars Müller[1,2,6], Diana Nanova[1,2,6], Tobias Glaser[2,6], Sebastian Beck[2,6], Annemarie Pucci[2,6], Anne K. Kast[3,6], Rasmus R. Schröder[3,4,6], Eric Mankel[5,6], Robert Lovrincic[1,6], and Wolfgang Kowalsky[1,2,6] — [1]IHF, TU Braunschweig — [2]KIP, Heidelberg University — [3]BioQuant, Heidelberg University — [4]CAM, Heidelberg University — [5]Surface Science Division, TU Darmstadt — [6]InnovationLab, Heidelberg

Doping of organic semiconductors is a prerequisite for the production of efficient devices such as organic light emitting diodes. Numerous recent publications reveal new insights on doping mechanisms and charge transfer, emphasizing the need for further investigations, especially on polymer systems. In this work, we study p-type doping of poly(3-hexylthiophene) (P3HT) with 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ), spin coated from the solvents chlorobenzene or chloroform. We find that films prepared from chloroform show a higher conductivity than films prepared from chlorobenzene. To clarify this unintuitive behavior, electron diffraction is used to reveal differences in the structural order within films from the two solvents. Additionally, UV-Vis and infrared spectroscopy help to expand the view to electronic properties such as vibrational or polaronic absorptions. It turns out that structural order and electronic properties in doped films are predefined by the interaction of the solvent with charge-transfer complexes already in solution.

CPP 63: Interfaces and Thin Films II (joint session CPP/DY, organized by CPP)

Time: Friday 9:30–12:00 Location: H51

CPP 63.1 Fri 9:30 H51

Ring polymer chains in confined geometries: Massive field theory approach — •Zoryana Usatenko[1] and Joanna Halun[2] — [1]Institute of Physics, Cracow University of Technology — [2]Faculty of Physics, Mathematics and Computer Science, Cracow University of Technology

The investigation of a dilute solution of phantom ideal and real ring polymer chains with excluded volume interactions in a good solvent confined in a slit geometry of two parallel walls was performed. Taking into account the well known polymer - magnet analogy developed by de Gennes the calculations of the correspondent partition functions, depletion interaction potentials, depletion forces and the forces which exert phantom ideal ring polymer chain on the surfaces were performed in a fixed space dimensions d=3 for two repulsive walls, two inert walls and for the mixed case of one inert and one repulsive wall. Besides, for the case of ring polymer chain with EVI confined in a slit geometry of two parallel repulsive walls calculations were performed up to one-loop order. It was found that the confining of ring polymer chain to a slit geometry of two walls leads to the loss of configurational entropy and to arising of the repulsive force which exerts ring polymer chain on the surfaces. Increasing of the slit size leads to decreasing of the value of the exerted force on the surfaces at the same value of the end-to-end distance.

CPP 63.2 Fri 9:45 H51

A theoretical approach to bis-urea molecules that form hydrogen-bonded supramolecular polymers in 2D — •Olga Guskova[1,2] and Jens-Uwe Sommer[1,2,3] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TU Dresden, Dresden, Germany — [3]Institute of Theoretical Physics, TU Dresden, Dresden, Germany

Supramolecular polymers, i.e. arrays of low-molecular-weight building blocks, usually held together by hydrogen bonding (HB) or other reversible noncovalent interactions. Bis-urea-based molecules with central bis-urea fragment exhibit the highest supramolecular polymerization ability, affording well-defined supramolecular fibers. In this talk, two major points concerning the arrangement and properties of HB bis-urea molecules on surfaces studied by QM/all-atom MD simulations will be addressed: (i) the ordering dynamics on graphite of two bis-urea molecules which differed only by a single cis-double bond in their side groups [1] and (ii) the electronic properties of isolated molecules, HB dimers and bis-urea tapes in adsorbed state on gold surface [2].

[1] R. Shokri, O. Guskova, A. Jamal, K. Jahanshahi, B. Isare, L. Bouteiller, L. Simon, J.-U. Sommer, G. Reiter, J. Phys. Chem. C 119 (39), 22596-22603 (2015).

[2] F. Vonau, R. Shokri, D. Aubel, L. Bouteiller, O. Guskova, J.-U. Sommer, G. Reiter, L. Simon, Nanoscale 6 (4), 8250-8256 (2014).

CPP 63.3 Fri 10:00 H51

Towards large area atomically flat n-alkane layers: A real-time study of thermal annealing — •Linus Pithan[1], Eduard Meister[2], Chenyu Jin[3], Anton Zykov[1], Wolfgang Brütting[2], Hans Riegler[3], Andreas Opitz[1], and Stefan Kowarik[1] — [1]Inst. f. Physik, Humboldt Universität zu Berlin — [2]Inst. f. Physik, Universität Augsburg — [3]MPI für Kolloid- und Grenzflächenforschung, Potsdam

Highly anisotropic attachment energies of n-alkanes combined with low surface energies result in their unusual thin films growth and wetting behavior [1]. We analyze the thermal annealing behavior of ntetratetracontane (TTC, $C_{44}H_{90}$) in detail with the aim to improve smoothness and to increase the lateral size of crystalline islands of polycrystalline TTC films on SiO, a material system also of interest from a device perspective [2]. We use *in situ* x-ray diffraction to find an optimum temperature leading to improved texture and crystallinity while avoiding an irreversible phase transition. Further, we employ real-time optical phase contrast microscopy with sub-nm height resolution [3] to track the diffusion of TTC across monomolecular step edges and show that the lateral island sizes increase by more than one order of magnitude from 0.5 μm to 10 μm. This desirable behavior of 2d-Ostwald ripening and the pronounced smoothing we observe is in stark contrast to many other organic molecular films where annealing leads to dewetting, roughening, and a pronounced 3d morphology.

[1] L. Pithan *et al.*, J. Chem. Phys. 143, 164707 (2015)
[2] M. Kraus *et al.*, J. Appl. Phys. 107, 094503 (2010)
[3] R. Köhler *et al.*, Appl. Phys. Lett. 89, 241906 (2006)

CPP 63.4 Fri 10:15 H51

Photo-manipulation of the surface tension anisotropy at a liquid-crystal/ITO-glass interface — Hajnalka Nadasi, •Alexey Eremin, and Ralf Stannarius — Institute of Experimental Physics, Otto von Guericke University Magdeburg, Universitätsplatz 2, 39016 Magdeburg, Germany

We report direct measurements of the surface energy anisotropy (anchoring energy) at a glass-nematic liquid crystal interface containing a photo-active azo-dendrimeric surfactant. The photoisomerisation at the surface layer drives an anchoring transition from the homogeneous to the planar sate of the liquid crystal. The anchoring energy is measured using the Frederiksz transition as a function of the intensities of the UV and VIS light and is compared with a theoretical model. We also demonstrate optical manipulation of the nematic director field around microshperes and rods dispersed in the liquid crystal. In case of rod-shaped particles, the photo-driven change of the anchoring energy results in a reversible macroscopic rotation of the particles.

CPP 63.5 Fri 10:30 H51

Kinetic Monte Carlo Simulations of Photo-Switchable Molecules Tethered to a Surface — •Raffaele Tavarone[1], Patrick Charbonneau[2], and Holger Stark[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Departments of Chemistry and Physics, Duke University, Durham, North Carolina 27708, USA

Photo-switchable molecules can undergo a light-induced *trans-cis* isomerization. They can be used to build functional monolayers with light-controlled macroscopic properties. A recent experiment [1] showed that, in a monolayer densely covered with photo-switchable molecules, the relaxation of the induced birefringence follows a glasslike power-law dynamics. Furthermore, the relaxation can be efficiently fastened by illumination of the sample with circularly polarized light.

We developed a molecular model for the monolayer in which the *trans* and *cis* isomers are modeled as straight and bent needles, respectively. The needles are allowed to overlap and the system dynamics is generated by a kinetic Monte Carlo algorithm. We demonstrate that the glasslike power-law dynamics can be traced back to spatio-temporal correlations in the local structure of the system, *i.e.*, to the formation of dynamical heterogeneities. Also, we find that the different degree of shape anisotropy of the two isomers has a significant effect on the system dynamics: the nearly isotropic *cis* isomers suppress the formation of extended dynamical domains. As a results, the relaxation is faster and follows a simple exponential decay.

[1] Fang, G. J., et al., Nature communications **4**, 1521 (2013).

15 min. break

CPP 63.6 Fri 11:00 H51

Modulated structures in complex twist-bend nematic phases in bulk and thin-film geometry. — •Nerea Sebastian, Alexey Eremin, and Ralf Stannarius — Institute of Experimental Physics, Otto von Guericke University Magdeburg, Universitätsplatz 2, 39016 Magdeburg, Germany

Twist-bend nematic state (Ntb) has recently been discovered as a complex mesophase intermediate between the cholesteric and a uniform nematic phase. The molecules, being non-chiral, spontaneously form a helical twist-bend structure, where the director is inclined to the helical axis. The phase is believed to be driven by the inversion of the bend elastic constant K3. We report on an elastic behaviour in the vicinity of the nematic-Ntb transition and describe the transition between the Ntb and a modulated smectic phase which exhibits intricate labyrinthine structures of the layer dislocations in freely-suspended films. It also forms fluid cylindrical filaments with large slenderness ratios.

The authors acknowledge the support by DFG (ER 467/8-1)

CPP 63.7 Fri 11:15 H51

Properties of a monomolecular water film flowing into a graphene-mica slit pore — •André Schilo, Nikolai Severin, Igor M. Sokolov, and Jürgen P. Rabe — Department of Physics, Humboldt-Universität zu Berlin, Germany

Nanoscopically confined water and water adsorbed at interfaces play an important role in e.g. biology, tribology or nanotechnology. Graphene has recently been demonstrated to replicate the substrate topography with a precision down to single macromolecules. Thus the flexible graphene cover provides the possibility of visualizing a water monolayer confined in a slit pore between graphene and mica. However, the phase of the confined water (solid or fluid) is still debated. Here we report high-resolution scanning force microscopy (SFM) imaging of water monolayers flowing into the slit pore. The initially dry pore gets filled upon raising the ambient humidity. We observed a layer of water wetting the sample in reproducible finger-shaped patterns with a step height of 2.8 Å. The flow kinetics are highly dependent on the rate of humidity change. Keeping the humidity constant at a value above the beginning of the wetting process and below the complete wetting, results in a nearly exponential saturation of the finger growth. A further increase of the humidity reactivates the growth of the fingers, eventually leading to a complete monolayer of water. From this we conclude that the confined water monolayer must be fluid.

CPP 63.8 Fri 11:30 H51

A spectroscopic investigation of surface melting of ice — •M.Alejandra Sanchez, Mischa Bonn, and Ellen H.G Backus — Max Planck Polymer Research Institute,Mainz,Germany

In nature, ice is, amongst others, responsible for rock weathering, soil metamorphosis, thunderstorms and the ozone chemistry on stratospheric clouds. It has been generally accepted that from the bulk freezing point down to roughly 240 K, a quasi-liquid-layer is present on ice. However, the nature of this layer has been intensely debated. We study the nature of the interfacial water on well-defined single crystal ice surfaces. The surface sensitive technique sum frequency generation spectroscopy provides the vibrational spectrum of specifically the interfacial molecules. We find a sudden change in the spectrum around 255 K which is assigned to the phase transition from ice/air to ice/quasi-liquid/air. The experimental results are well reproduced by simulations that allow to relate the observed spectral changes to information on the molecular scale.

CPP 63.9 Fri 11:45 H51

Interfacial Melting in Ice/Nanocomposite Materials — •Hailong Li[1], Julian Mars[1,2], Henning Weiss[1], Thomas Buslaps[3], Wiebke Lohstroh[4], and Markus Mezger[1,2] — [1]Max-Planck-Institut für Polymerforschung, Mainz, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany — [3]ESRF-The European Synchrotron, Grenoble, France — [4]Heinz Maier-Leibnitz Zentrum, Technische Universität München, Germany

The material properties of permafrost strongly depend on the molecular scale structure of the ice/solid interface. Early in 1859, Faraday proposed the existence of a quasi-liquid layer (qll) at ice surfaces. However, the understanding of the interfacial melting of ice and the structure of the qll is still under debate. Layered sheet silicates are ideal model systems to study the interfacial melting of ice in geologically relevant materials. Using x-ray diffraction, we determined the crystalline ice fraction in ice composites with high interface to volume ratio. From the anisotropy of the ice Bragg reflections in textured composite samples we extract the preferred orientation of ice crystals confined between the sheet silicates. Approaching the bulk melting point of ice, we observe a logarithmic growth law of the thickness of the qll. Quasielastic neutron scattering was employed to elucidate the mobility of the qll at hydrophilic and hydrophobic solid-ice interfaces.